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## The Chemkin Thermodynamic Data Base

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## THE CHEMKIN THERMODYNAMIC DATA BASE

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### Abstract

The Chemkin general-purpose chemical kinetics package uses a data base that contains polynomial fits to specific heats, standard state enthalpies, and standard state entropies. The fourteen coefficient fits are in the same form as used in the NASA Complex Chemical Equilibrium Program (Gordon and McBride, 1971). This report represents a compilation of the data that is currently in use at Sandia National Laboratories.

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## THE CHEMKIN THERMODYNAMIC DATA BASE

### Introduction

This report documents the thermodynamic property data base that is an integral part of the Chemkin<sup>1,2</sup> chemical kinetics computer code package. The codes are documented in user's manuals. However, a brief description of the package's structure may help put the role of the data base in perspective. Chemkin is composed of four important pieces: the Interpreter, the Thermodynamic Data Base, the Linking File, and the Gas-Phase Subroutine Library. The Interpreter is a program that first reads the user's symbolic description of the reaction mechanism. It then extracts thermodynamic information for the species involved from the Thermodynamic Data Base. The user may add to or modify the information in the data base by input to the Interpreter. In addition to printed output, the Interpreter writes a Linking File, which contains all the pertinent information on the elements, species, and reactions in the mechanism.

Once the Interpreter has been executed and the Linking File created, the user is ready to use the Gas-Phase Subroutine Library. These subroutines are called from the user's Fortran code. The Chemkin gas-phase subroutines, of which there are over 100, are called as needed to return information on the elements, species, reactions, equations of state, thermodynamic properties, chemical production rates, sensitivity parameters, derivatives of chemical production rates, and derivatives of thermodynamic properties. Generally the input to these routines is the state of the gas – pressure or density, temperature, and the species composition. The Chemkin documentation is designed to facilitate selection of the particular Chemkin subroutines that are needed for a given problem.

We developed the Chemkin package and its follow-on applications programs for use in our combustion research programs. Our combustion work concentrates on small molecule hydrocarbon systems, especially those involving the nitrogen chemistry responsible for producing nitrogen-oxygen based pollutants. Thus we have gathered thermodynamic properties for the species important in such systems. Moreover, because of our investigations of the chemical vapor deposition of silicon from silane, the data base includes several silicon-hydrogen compounds. It was not our intent to make wide distribution of these codes or data bases. However, over the past several years, the code package has found rather wide acceptance.

As part of the Chemkin code distribution process, we have supplied its associated thermodynamic data base. However, this was done in an unstructured way. That is, recipients of the data base had no way to tell where the data came from or any information about its validity. The data base was simply the one that was in use at Sandia at the time the tape was written. Since, a great many Chemkin simulations are finding their way into the literature, we decided that it would be a good idea to document the data base. However, our basic motivation remains unchanged. We maintain the data base for our own research programs, and we in no way see ourselves as a clearinghouse for property data or as competitors with JANAF or the National Bureau of Standards. Nevertheless, for certain classes of problems, we believe that sharing our thermodynamic data compilation could prove valuable in other research programs.

In this report, we first explain how the polynomial fits to the property data are generated. Then in three appendices we present the data itself in several formats. Appendix A lists the standard state heats of formation and entropies at 298K for each of the species in the data base. Appendix B is a listing of the data base in the form that Chemkin expects to find it. Finally, Appendix C presents a graphical account of the properties as a function of temperature. Where available, the actual data from which the fits were determined are also plotted to indicate the accuracy of the fit. Also in this section a reference to the source of the data is provided.

### The data sources

The data comes from three major sources. First is the JANAF<sup>3</sup> tables. Generally speaking, if available, JANAF is the preferred source of our data. The properties of many hydrocarbon species not included in the JANAF compilations come from the compilation of Burcat.<sup>4</sup> In this case, the data provided by Burcat is already fit in the form required for our data base. The third source of data is quantum chemistry computations.

Calculation of thermochemical data using high-quality *ab initio* electronic structure calculations has been a long-standing goal. However, the availability of supercomputers and new theoretical techniques now allow the calculation of thermochemical properties with chemical accuracy, i.e.,  $\Delta H_f$  to within  $\pm 3$  kcal/mole. A technique that has been applied to over 900 combustion-related chemical species and to our study of silicon-containing species is denoted the BAC-MP4 method.<sup>5-9</sup> It combines electronic structure calculations using fourth-order Møller-Plesset perturbation theory<sup>10-12</sup> (MP4) with empirically-derived bond additivity correction (BAC) factors to account for systematic error in the *ab initio* calculations due to truncated wave functions and incomplete basis sets.

## The fitting procedure

The data format used is a minor modification of that used by Gordon and McBride<sup>13</sup> for the thermodynamic data base in the NASA Chemical Equilibrium program. The thermodynamic data are stored as polynomial fits to specific heat  $c_p/R$ , enthalpy  $H^0/RT$ , and entropy  $S^0/R$ . There are seven coefficients for each of two temperature ranges.

$$\frac{c_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \quad (1)$$

$$\frac{H^0}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T} \quad (2)$$

$$\frac{S^0}{R} = a_1 \ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7 \quad (3)$$

Thus for each species there are 14 coefficients in all. In addition to the polynomial coefficients for each species, the Thermodynamic Data Base provides the species name, its elemental makeup, and the temperature ranges over which the fits are valid.

The essential input to the fitting procedure is a table of specific heat, enthalpy, and entropy as a function of temperature. In addition, since the fits span two temperature ranges, the temperature ranges have to be specified. Generally speaking, the common temperature connecting the two ranges is 1000K, but it may be different in some cases.

The constrained linear least squares fitting procedure<sup>14,15</sup> is a three stage process. The first step is to determine simultaneously  $a_1$  through  $a_5$  for both temperature ranges by fitting the specific heats Eq. (1). The fitting procedure is constrained such that at the common temperature both the specific heat and its first derivative are equal. The second step is to determine  $a_6$  for both temperature ranges by fitting the enthalpy data. In this stage,  $a_1 - a_5$  are held fixed, and as in the  $c_p$  fitting, equality constraints on the fit and its first derivative are imposed at the common temperature. Finally, the  $a_7$  coefficients are determined by fitting the entropy data. Again, the  $a_1 - a_5$  coefficients are held fixed and the equality constraints are imposed at the common temperature. We note that this fitting procedure is slightly different from the procedure followed by McBride and Gordon,<sup>16</sup> who fit all coefficients simultaneously.

## Data base management

The Chemkin data base requires a four card image fixed format representation of the properties for each species. This is consistent with other data bases, such as that used in the NASA Chemical Equilibrium Code.<sup>13</sup> However, while this format is complete enough to describe the properties, it contains only the bare minimum data needed. Therefore, we now maintain the data base using a relational data base manager program called DATA-TRIEVE, which is a proprietary product of the Digital Equipment Corporation (DEC).



The data base contains the following fields:

1. Identification - chemical symbol, species name, elemental composition, and phase;
2. Fit coefficients for the thermodynamic properties, and the temperature ranges for which they apply.
3. Data used to generate the fit, if available. These fields contain  $H^0(298)$ ,  $S^0(298)$ , and tables of  $c_p(T)$ ,  $S^0(T)$ ,  $H^0(T)$  as functions of temperature.
4. References - source of data, date, any relevant comments.

Using a relational data base manager provides considerably more flexibility in managing the data than the original Chemkin data base. Various types of reports can be produced from database manager program. The appendices in this report represent three examples of such reports. The data base that Chemkin uses is simply one of the reports from the DATATRIEVE system.

#### Acknowledgement

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# APPENDIX A. STANDARD STATE ENTHALPIES AND ENTROPIES AT 298K

TABLE A1.

| Species                             | H <sup>0</sup> (298)<br>Kcal/mole | S <sup>0</sup> (298)<br>cal/mole K | Species                              | H <sup>0</sup> (298)<br>Kcal/mole | S <sup>0</sup> (298)<br>cal/mole K |
|-------------------------------------|-----------------------------------|------------------------------------|--------------------------------------|-----------------------------------|------------------------------------|
| <i>Al</i>                           | 78.77                             | 39.29                              | <i>C<sub>2</sub>HCl</i>              | 51.08                             | 57.80                              |
| <i>Al<sub>2</sub>H<sub>6</sub></i>  | 21.34                             | 62.73                              | <i>C<sub>2</sub>N</i>                | 132.95                            | 55.13                              |
| <i>Al<sub>2</sub>Me<sub>6</sub></i> | -61.17                            | 131.01                             | <i>C<sub>2</sub>N<sub>2</sub></i>    | 73.84                             | 57.69                              |
| <i>AlAs</i>                         | 107.28                            | 60.63                              | <i>C<sub>2</sub>O</i>                | 68.47                             | 55.65                              |
| <i>AlH</i>                          | 61.97                             | 44.85                              | <i>C<sub>3</sub></i>                 | 195.92                            | 56.64                              |
| <i>AlH<sub>2</sub></i>              | 41.93                             | 54.38                              | <i>C<sub>3</sub>H<sub>2</sub></i>    | 106.47                            | 56.19                              |
| <i>AlH<sub>3</sub></i>              | 18.82                             | 52.28                              | <i>C<sub>3</sub>H<sub>4</sub></i>    | 45.21                             | 54.87                              |
| <i>AlMe</i>                         | 19.74                             | 60.65                              | <i>C<sub>3</sub>H<sub>4</sub>C</i>   | 66.17                             | 58.16                              |
| <i>AlMe<sub>2</sub></i>             | 12.75                             | 77.37                              | <i>C<sub>3</sub>H<sub>4</sub>P</i>   | 43.95                             | 49.47                              |
| <i>AlMe<sub>3</sub></i>             | -20.29                            | 83.65                              | <i>C<sub>3</sub>H<sub>6</sub></i>    | 4.88                              | 61.48                              |
| <i>Ar</i>                           | 0.00                              | 36.96                              | <i>C<sub>3</sub>H<sub>8</sub></i>    | -24.81                            | 64.53                              |
| <i>Ar<sup>+</sup></i>               | 364.76                            | 39.73                              | <i>C<sub>3</sub>O<sub>2</sub></i>    | -22.37                            | 65.94                              |
| <i>As</i>                           | 75.45                             | 43.51                              | <i>C<sub>4</sub></i>                 | 231.91                            | 54.53                              |
| <i>As<sub>2</sub></i>               | 47.06                             | 59.80                              | <i>C<sub>4</sub>H</i>                | 155.02                            | 60.86                              |
| <i>As<sub>3</sub></i>               | 65.32                             | 77.49                              | <i>C<sub>4</sub>H<sub>2</sub></i>    | 111.66                            | 59.75                              |
| <i>As<sub>4</sub></i>               | 37.11                             | 78.42                              | <i>C<sub>4</sub>H<sub>6</sub></i>    | 34.95                             | 68.13                              |
| <i>AsAlMe</i>                       | 69.97                             | 81.57                              | <i>C<sub>4</sub>H<sub>8</sub></i>    | -0.13                             | 73.52                              |
| <i>AsAlMe<sub>2</sub></i>           | 63.23                             | 90.97                              | <i>C<sub>5</sub></i>                 | 233.91                            | 57.80                              |
| <i>AsGaEt</i>                       | 82.72                             | 95.17                              | <i>C<sub>5</sub>H</i>                | 185.92                            | 62.18                              |
| <i>AsGaEt<sub>2</sub></i>           | 69.52                             | 109.79                             | <i>C<sub>5</sub>H<sub>12</sub></i>   | -34.96                            | 83.45                              |
| <i>AsGaMe</i>                       | 83.47                             | 85.72                              | <i>C<sub>5</sub>H<sub>2</sub></i>    | 165.17                            | 63.66                              |
| <i>AsGaMe<sub>2</sub></i>           | 81.22                             | 90.97                              | <i>C<sub>5</sub>H<sub>3</sub></i>    | 135.36                            | 70.50                              |
| <i>AsGaMeH</i>                      | 93.71                             | 84.69                              | <i>C<sub>5</sub>H<sub>6</sub></i>    | 31.98                             | 64.42                              |
| <i>AsH</i>                          | 61.73                             | 50.18                              | <i>C<sub>6</sub>H</i>                | 213.07                            | 74.07                              |
| <i>AsH<sub>2</sub></i>              | 42.23                             | 46.43                              | <i>C<sub>6</sub>H<sub>10</sub></i>   | -1.00                             | 74.72                              |
| <i>AsH<sub>3</sub></i>              | 16.62                             | 55.63                              | <i>C<sub>6</sub>H<sub>14</sub></i>   | -39.89                            | 92.84                              |
| <i>AsMe</i>                         | 59.18                             | 63.78                              | <i>C<sub>6</sub>H<sub>2</sub></i>    | 169.59                            | 70.89                              |
| <i>AsMe<sub>2</sub></i>             | 34.19                             | 79.47                              | <i>C<sub>6</sub>H<sub>3</sub></i>    | 158.38                            | 76.26                              |
| <i>AsMe<sub>3</sub></i>             | 2.92                              | 85.74                              | <i>C<sub>6</sub>H<sub>4</sub></i>    | 121.72                            | 69.51                              |
| <i>C</i>                            | 171.22                            | 37.74                              | <i>C<sub>6</sub>H<sub>5</sub></i>    | 79.40                             | 69.79                              |
| <i>C(S)</i>                         | 0.00                              | 1.37                               | <i>C<sub>6</sub>H<sub>5</sub>(L)</i> | 140.52                            | 84.23                              |
| <i>C<sup>+</sup></i>                | 431.85                            | 36.92                              | <i>C<sub>6</sub>H<sub>5</sub>O</i>   | 10.35                             | 74.84                              |
| <i>C<sup>-</sup></i>                | 140.55                            | 36.14                              | <i>C<sub>6</sub>H<sub>5</sub>OH</i>  | -25.00                            | 76.90                              |
| <i>C<sub>2</sub></i>                | 200.15                            | 47.61                              | <i>C<sub>6</sub>H<sub>6</sub></i>    | 19.80                             | 64.33                              |
| <i>C<sub>2</sub><sup>-</sup></i>    | 105.96                            | 46.94                              | <i>C<sub>6</sub>H<sub>7</sub></i>    | 47.94                             | 73.05                              |
| <i>C<sub>2</sub>F<sub>6</sub></i>   | -321.07                           | 79.35                              | <i>C<sub>8</sub>H</i>                | 288.74                            | 78.35                              |
| <i>C<sub>2</sub>H</i>               | 133.95                            | 49.54                              | <i>C<sub>8</sub>H<sub>2</sub></i>    | 226.06                            | 75.91                              |
| <i>C<sub>2</sub>H<sub>2</sub></i>   | 54.17                             | 47.99                              | <i>CCL</i>                           | 119.95                            | 53.61                              |
| <i>C<sub>2</sub>H<sub>3</sub></i>   | 68.38                             | 55.30                              | <i>CCl<sub>2</sub></i>               | 56.98                             | 63.36                              |
| <i>C<sub>2</sub>H<sub>4</sub></i>   | 12.53                             | 52.35                              | <i>CCl<sub>3</sub></i>               | 18.99                             | 70.90                              |
| <i>C<sub>2</sub>H<sub>5</sub></i>   | 28.00                             | 60.11                              | <i>CCl<sub>4</sub></i>               | -22.93                            | 74.01                              |
| <i>C<sub>2</sub>H<sub>6</sub></i>   | -20.03                            | 54.69                              | <i>CH</i>                            | 141.94                            | 43.70                              |

TABLE A1. (continued)

| Species                             | H <sup>0</sup> (298)<br>Kcal/mole | S <sup>0</sup> (298)<br>cal/mole K | Species                            | H <sup>0</sup> (298)<br>Kcal/mole | S <sup>0</sup> (298)<br>cal/mole K |
|-------------------------------------|-----------------------------------|------------------------------------|------------------------------------|-----------------------------------|------------------------------------|
| CH <sup>+</sup>                     | 388.65                            | 40.98                              | CO <sub>2</sub> <sup>-</sup>       | -105.46                           | 57.46                              |
| CH <sub>2</sub>                     | 92.45                             | 46.69                              | CO <sub>2</sub> S                  | -33.07                            | 55.30                              |
| CH <sub>2</sub> (S)                 | 101.46                            | 45.08                              | CS                                 | 66.97                             | 50.27                              |
| CH <sub>2</sub> CHCCH               | 69.11                             | 67.30                              | CS <sub>2</sub>                    | 27.94                             | 56.83                              |
| CH <sub>2</sub> CHCCH <sub>2</sub>  | 74.11                             | 75.28                              | E                                  | 0.00                              | 4.98                               |
| CH <sub>2</sub> CHCH <sub>2</sub>   | 38.62                             | 64.71                              | F                                  | 18.85                             | 37.90                              |
| CH <sub>2</sub> CHCHCH              | 86.06                             | 73.04                              | F <sub>2</sub>                     | 0.00                              | 48.42                              |
| CH <sub>2</sub> CHCHCH <sub>2</sub> | 28.28                             | 70.41                              | F <sub>2</sub> SiNH                | -146.87                           | 70.89                              |
| CH <sub>2</sub> Cl <sub>2</sub>     | -22.82                            | 64.54                              | F <sub>3</sub> SiN                 | -199.94                           | 73.84                              |
| CH <sub>2</sub> CO                  | -12.39                            | 57.76                              | FNNF                               | 17.87                             | 63.44                              |
| CH <sub>2</sub> F <sub>2</sub>      | -107.67                           | 58.89                              | FNO <sub>3</sub>                   | 2.50                              | 69.96                              |
| CH <sub>2</sub> HCO                 | 5.99                              | 63.97                              | FO                                 | 25.99                             | 51.74                              |
| CH <sub>2</sub> O                   | -27.69                            | 52.22                              | FO <sub>2</sub>                    | 3.00                              | 61.88                              |
| CH <sub>2</sub> OH                  | -4.10                             | 58.85                              | FSiN                               | 54.35                             | 63.64                              |
| CH <sub>3</sub>                     | 34.80                             | 46.35                              | Ga                                 | 68.50                             | 43.81                              |
| CH <sub>3</sub> CC                  | 123.77                            | 60.25                              | Ga <sub>2</sub> H <sub>6</sub>     | 31.49                             | 69.03                              |
| CH <sub>3</sub> CCCH <sub>2</sub>   | 74.31                             | 80.32                              | GaAs                               | 88.37                             | 63.20                              |
| CH <sub>3</sub> CCCH <sub>3</sub>   | 40.92                             | 73.33                              | GaAs(3,C)                          | 245.65                            | 99.96                              |
| CH <sub>3</sub> CCH <sub>2</sub>    | 61.06                             | 69.22                              | GaAs(3,L)                          | 256.15                            | 127.70                             |
| CH <sub>3</sub> CH <sub>2</sub> CCH | 44.73                             | 71.41                              | GaAs(5,C)                          | 357.61                            | 130.45                             |
| CH <sub>3</sub> CHCH                | 64.72                             | 68.71                              | GaAs(5,L)                          | 419.83                            | 193.42                             |
| CH <sub>3</sub> Cl                  | -19.99                            | 55.95                              | GaEt                               | 17.74                             | 81.57                              |
| CH <sub>3</sub> CO                  | -5.40                             | 63.71                              | GaEt <sub>2</sub>                  | 4.50                              | 100.39                             |
| CH <sub>3</sub> F                   | -55.98                            | 53.20                              | GaEt <sub>3</sub>                  | -17.04                            | 112.94                             |
| CH <sub>3</sub> HCO                 | -39.49                            | 63.02                              | GaH                                | 54.78                             | 49.16                              |
| CH <sub>3</sub> O                   | 3.89                              | 54.58                              | GaH <sub>2</sub>                   | 40.98                             | 55.98                              |
| CH <sub>3</sub> OH                  | -48.04                            | 57.24                              | GaH <sub>3</sub>                   | 26.99                             | 54.48                              |
| CH <sub>3</sub> SiCl <sub>3</sub>   | -126.35                           | 83.85                              | GaMe                               | 18.52                             | 63.78                              |
| CH <sub>4</sub>                     | -17.89                            | 44.44                              | GaMe <sub>2</sub>                  | 16.42                             | 80.52                              |
| CHCl                                | 79.97                             | 56.09                              | GaMe <sub>3</sub>                  | -10.87                            | 87.84                              |
| CHCl <sub>3</sub>                   | -24.65                            | 70.60                              | H                                  | 52.07                             | 27.38                              |
| CHF                                 | 29.99                             | 53.33                              | H <sup>+</sup>                     | 367.01                            | 26.00                              |
| CHF <sub>3</sub>                    | -166.54                           | 62.00                              | H <sup>-</sup>                     | 33.18                             | 26.00                              |
| Cl                                  | 28.98                             | 39.44                              | H <sub>2</sub>                     | 0.00                              | 31.19                              |
| Cl <sub>2</sub>                     | 0.00                              | 53.27                              | H <sub>2</sub> AlMe                | 6.00                              | 61.70                              |
| CN                                  | 103.96                            | 48.38                              | H <sub>2</sub> AsMe                | 24.04                             | 64.83                              |
| CN <sup>+</sup>                     | 430.70                            | 50.96                              | H <sub>2</sub> C <sub>4</sub> O    | 54.57                             | 66.40                              |
| CN <sup>-</sup>                     | 14.49                             | 46.79                              | H <sub>2</sub> CCCCCH              | 111.27                            | 72.91                              |
| CN <sub>2</sub>                     | 112.95                            | 54.01                              | H <sub>2</sub> CCCCCH <sub>2</sub> | 75.46                             | 65.10                              |
| CNN                                 | 139.64                            | 55.33                              | H <sub>2</sub> CCCCH               | 83.00                             | 61.45                              |
| CO                                  | -26.41                            | 47.19                              | H <sub>2</sub> CN                  | 59.08                             | 53.57                              |
| CO <sub>2</sub>                     | -94.01                            | 51.05                              | H <sub>2</sub> CNH                 | 21.84                             | 55.43                              |

TABLE A1. (continued)

| Species                                            | H <sup>0</sup> (298)<br>Kcal/mole | S <sup>0</sup> (298)<br>cal/mole K | Species                                | H <sup>0</sup> (298)<br>Kcal/mole | S <sup>0</sup> (298)<br>cal/mole K |
|----------------------------------------------------|-----------------------------------|------------------------------------|----------------------------------------|-----------------------------------|------------------------------------|
| <i>H<sub>2</sub>CNNO<sub>2</sub></i>               | 33.63                             | 73.03                              | <i>HGaMe</i>                           | 28.99                             | 65.88                              |
| <i>H<sub>2</sub>GaEt</i>                           | -2.30                             | 83.65                              | <i>HGaMe<sub>2</sub></i>               | 2.50                              | 79.47                              |
| <i>H<sub>2</sub>GaMe</i>                           | 14.99                             | 64.83                              | <i>HMeGaEt</i>                         | 4.00                              | 88.87                              |
| <i>H<sub>2</sub>NF</i>                             | -6.49                             | 54.70                              | <i>HN<sub>3</sub></i>                  | 71.84                             | 57.12                              |
| <i>H<sub>2</sub>O</i>                              | -57.78                            | 45.08                              | <i>HNCO</i>                            | -24.89                            | 57.03                              |
| <i>H<sub>2</sub>O(L)</i>                           | -68.29                            | 16.70                              | <i>HN<sub>2</sub>F</i>                 | 31.98                             | 54.95                              |
| <i>H<sub>2</sub>O(S)</i>                           | -69.93                            | 10.70                              | <i>HN<sub>2</sub>F<sub>2</sub></i>     | -13.79                            | 60.03                              |
| <i>H<sub>2</sub>O<sub>2</sub></i>                  | -32.52                            | 55.63                              | <i>HNO</i>                             | 23.79                             | 52.70                              |
| <i>H<sub>2</sub>S</i>                              | -4.90                             | 49.12                              | <i>HNO<sub>3</sub></i>                 | -32.09                            | 63.64                              |
| <i>H<sub>2</sub>Si(NH<sub>2</sub>)<sub>2</sub></i> | -37.14                            | 72.35                              | <i>HO<sub>2</sub></i>                  | 2.50                              | 54.70                              |
| <i>H<sub>2</sub>SiN</i>                            | 149.13                            | 59.49                              | <i>HOCN</i>                            | -2.28                             | 59.21                              |
| <i>H<sub>2</sub>SiNH</i>                           | 40.94                             | 60.07                              | <i>HONO</i>                            | -18.33                            | 59.56                              |
| <i>H<sub>2</sub>SiNH<sub>2</sub></i>               | 28.08                             | 65.76                              | <i>HSi(NH<sub>2</sub>)<sub>2</sub></i> | 5.76                              | 73.35                              |
| <i>H<sub>2</sub>SiNH<sub>3</sub></i>               | 23.84                             | 66.76                              | <i>HSi(NH<sub>2</sub>)<sub>3</sub></i> | -64.65                            | 79.49                              |
| <i>H<sub>2</sub>SiSiH<sub>2</sub></i>              | 62.84                             | 66.87                              | <i>HSiCl</i>                           | 16.99                             | 59.77                              |
| <i>H<sub>3</sub>AsGaEt<sub>3</sub></i>             | -10.99                            | 124.43                             | <i>HSiN</i>                            | 92.95                             | 54.73                              |
| <i>H<sub>3</sub>AsGaMe<sub>3</sub></i>             | -4.70                             | 102.46                             | <i>HSiNH</i>                           | 84.75                             | 60.66                              |
| <i>H<sub>3</sub>SiN</i>                            | 234.51                            | 56.91                              | <i>HSiNH<sub>2</sub></i>               | 26.28                             | 60.03                              |
| <i>H<sub>3</sub>SiNH</i>                           | 51.32                             | 66.19                              | <i>I * C<sub>3</sub>H<sub>7</sub></i>  | 18.19                             | 60.07                              |
| <i>H<sub>3</sub>SiSiH</i>                          | 80.17                             | 66.84                              | <i>Me<sub>2</sub>GaEt</i>              | -5.25                             | 97.24                              |
| <i>H<sub>3</sub>SiSiH<sub>3</sub></i>              | 19.16                             | 68.03                              | <i>MeGaEt</i>                          | 14.25                             | 89.92                              |
| <i>HAlMe</i>                                       | 27.24                             | 62.75                              | <i>MeGaEt<sub>2</sub></i>              | -7.32                             | 106.66                             |
| <i>HAlMe<sub>2</sub></i>                           | -6.72                             | 75.30                              | <i>N</i>                               | 112.90                            | 36.59                              |
| <i>HAsAlMe</i>                                     | 56.48                             | 83.64                              | <i>N * C<sub>3</sub>H<sub>7</sub></i>  | 22.59                             | 64.10                              |
| <i>HAsGaEt</i>                                     | 69.12                             | 97.24                              | <i>N<sub>2</sub></i>                   | 0.00                              | 45.75                              |
| <i>HAsGaMe</i>                                     | 69.97                             | 87.84                              | <i>N<sub>2</sub>H<sub>2</sub></i>      | 50.88                             | 52.18                              |
| <i>HAsMe</i>                                       | 42.56                             | 65.88                              | <i>N<sub>2</sub>H<sub>3</sub></i>      | 36.77                             | 54.59                              |
| <i>HAsMe<sub>2</sub></i>                           | 18.09                             | 78.42                              | <i>N<sub>2</sub>H<sub>4</sub></i>      | 22.78                             | 57.00                              |
| <i>HCCHCCH</i>                                     | 129.83                            | 69.03                              | <i>N<sub>2</sub>H<sub>4</sub>(L)</i>   | 12.09                             | 29.02                              |
| <i>HCCO</i>                                        | 42.43                             | 60.71                              | <i>N<sub>2</sub>O</i>                  | 19.60                             | 52.52                              |
| <i>HCCOH</i>                                       | 20.42                             | 58.67                              | <i>N<sub>2</sub>O<sup>+</sup></i>      | 318.56                            | 55.84                              |
| <i>HCl</i>                                         | -22.06                            | 44.62                              | <i>N<sub>2</sub>O<sub>4</sub></i>      | 2.17                              | 72.70                              |
| <i>HCN</i>                                         | 32.29                             | 48.19                              | <i>N<sub>3</sub></i>                   | 98.96                             | 54.08                              |
| <i>HCNH</i>                                        | 66.08                             | 55.87                              | <i>NCO</i>                             | 38.08                             | 55.45                              |
| <i>HCNO</i>                                        | 38.41                             | 53.77                              | <i>NF</i>                              | 59.47                             | 51.40                              |
| <i>HCO</i>                                         | 10.39                             | 53.63                              | <i>NFO</i>                             | -15.69                            | 59.25                              |
| <i>HCO<sup>+</sup></i>                             | 199.02                            | 48.57                              | <i>NFO<sub>2</sub></i>                 | -25.99                            | 62.15                              |
| <i>He</i>                                          | 0.00                              | 30.11                              | <i>NH</i>                              | 85.17                             | 43.27                              |
| <i>He<sup>+</sup></i>                              | 568.23                            | 31.48                              | <i>NH<sub>2</sub></i>                  | 45.48                             | 46.48                              |
| <i>HF</i>                                          | -65.12                            | 41.49                              | <i>NH<sub>3</sub></i>                  | -10.97                            | 46.01                              |
| <i>HGaEt</i>                                       | 22.89                             | 83.64                              | <i>NNH</i>                             | 58.54                             | 53.60                              |
| <i>HGaEt<sub>2</sub></i>                           | -2.30                             | 100.46                             | <i>NO</i>                              | 21.57                             | 50.32                              |

TABLE A1. (continued)

| Species                                                   | H <sup>0</sup> (298)<br>Kcal/mole | S <sup>0</sup> (298)<br>cal/mole K | Species                                            | H <sup>0</sup> (298)<br>Kcal/mole | S <sup>0</sup> (298)<br>cal/mole K |
|-----------------------------------------------------------|-----------------------------------|------------------------------------|----------------------------------------------------|-----------------------------------|------------------------------------|
| <i>NO</i> <sup>+</sup>                                    | 236.57                            | 47.32                              | <i>SiCl<sub>3</sub>H</i>                           | -118.55                           | 74.87                              |
| <i>NO</i> <sub>2</sub>                                    | 7.91                              | 57.31                              | <i>SiCl<sub>4</sub></i>                            | -158.34                           | 79.06                              |
| <i>NO</i> <sub>2</sub> <sup>-</sup>                       | -48.43                            | 56.49                              | <i>SiClH<sub>3</sub></i>                           | -32.19                            | 59.77                              |
| <i>NO</i> <sub>3</sub>                                    | 16.99                             | 60.33                              | <i>SiF</i>                                         | -12.41                            | 52.69                              |
| <i>O</i>                                                  | 59.53                             | 38.45                              | <i>SiF(NH<sub>2</sub>)<sub>2</sub></i>             | -95.30                            | 77.67                              |
| <i>O</i> <sup>+</sup>                                     | 374.80                            | 36.99                              | <i>SiF(NH<sub>2</sub>)<sub>3</sub></i>             | -170.48                           | 87.88                              |
| <i>O</i> <sup>-</sup>                                     | 24.31                             | 37.67                              | <i>SiF<sub>2</sub></i>                             | -149.80                           | 61.36                              |
| <i>O</i> <sub>2</sub>                                     | 0.00                              | 48.98                              | <i>SiF<sub>2</sub>(NH<sub>2</sub>)<sub>2</sub></i> | -247.09                           | 82.74                              |
| <i>O</i> <sub>2</sub> <sup>-</sup>                        | -11.61                            | 50.04                              | <i>SiF<sub>2</sub>N</i>                            | -63.08                            | 70.48                              |
| <i>O</i> <sub>3</sub>                                     | 34.09                             | 57.05                              | <i>SiF<sub>2</sub>NH<sub>2</sub></i>               | -167.14                           | 77.45                              |
| <i>OH</i>                                                 | 9.31                              | 43.86                              | <i>SiF<sub>3</sub></i>                             | -237.33                           | 67.74                              |
| <i>OH</i> <sup>+</sup>                                    | 314.67                            | 43.64                              | <i>SiF<sub>3</sub>NH</i>                           | -249.55                           | 83.66                              |
| <i>OH</i> <sup>-</sup>                                    | -34.31                            | 41.17                              | <i>SiF<sub>3</sub>NH<sub>2</sub></i>               | -317.76                           | 81.00                              |
| <i>S</i>                                                  | 66.17                             | 40.07                              | <i>SiF<sub>3</sub>NHSiH<sub>3</sub></i>            | -320.04                           | 96.84                              |
| <i>S(L)</i>                                               | 0.44                              | 8.77                               | <i>SiF<sub>3</sub>NSiH<sub>3</sub></i>             | -252.73                           | 99.30                              |
| <i>S(S)</i>                                               | 0.00                              | 7.62                               | <i>SiF<sub>4</sub></i>                             | -385.83                           | 67.52                              |
| <i>S</i> <sup>+</sup>                                     | 306.35                            | 39.06                              | <i>SiFH<sub>3</sub></i>                            | -85.47                            | 56.98                              |
| <i>S - Triazine</i>                                       | 56.35                             | 64.46                              | <i>SiFNH</i>                                       | -13.48                            | 68.92                              |
| <i>S</i> <sub>2</sub>                                     | 30.70                             | 54.48                              | <i>SiFNH<sub>2</sub></i>                           | -80.01                            | 64.59                              |
| <i>SH</i>                                                 | 33.29                             | 46.71                              | <i>SiH</i>                                         | 91.66                             | 44.18                              |
| <i>Si</i>                                                 | 107.66                            | 40.10                              | <i>SiH<sub>2</sub></i>                             | 64.77                             | 49.47                              |
| <i>Si(L)</i>                                              | 11.58                             | 10.62                              | <i>SiH<sub>2</sub>Cl</i>                           | 7.80                              | 62.27                              |
| <i>Si(NH<sub>2</sub>)<sub>3</sub></i>                     | -18.62                            | 84.24                              | <i>SiH<sub>2</sub>F</i>                            | -42.15                            | 59.68                              |
| <i>Si(NH<sub>2</sub>)<sub>4</sub></i>                     | -92.63                            | 85.34                              | <i>SiH<sub>2</sub>F<sub>2</sub></i>                | -186.31                           | 62.78                              |
| <i>Si(S)</i>                                              | 0.00                              | 4.50                               | <i>SiH<sub>3</sub></i>                             | 47.41                             | 51.78                              |
| <i>Si</i> <sub>2</sub>                                    | 140.94                            | 54.87                              | <i>SiH<sub>3</sub>NH<sub>2</sub></i>               | -11.39                            | 65.64                              |
| <i>Si</i> <sub>2</sub> <i>C</i>                           | 127.95                            | 57.86                              | <i>SiH<sub>3</sub>NHSiH<sub>3</sub></i>            | -14.31                            | 85.92                              |
| <i>Si</i> <sub>2</sub> <i>F</i> <sub>6</sub>              | -569.38                           | 97.12                              | <i>SiH<sub>3</sub>NSiH<sub>3</sub></i>             | 48.88                             | 86.66                              |
| <i>Si</i> <sub>2</sub> <i>H</i> <sub>2</sub>              | 83.46                             | 58.53                              | <i>SiH<sub>4</sub></i>                             | 8.10                              | 48.88                              |
| <i>Si</i> <sub>2</sub> <i>H</i> <sub>3</sub>              | 105.66                            | 65.48                              | <i>SiHCl<sub>2</sub></i>                           | -34.29                            | 70.27                              |
| <i>Si</i> <sub>2</sub> <i>H</i> <sub>5</sub>              | 55.68                             | 68.82                              | <i>SiHF</i>                                        | -35.69                            | 57.04                              |
| <i>Si</i> <sub>2</sub> <i>H</i> <sub>6</sub>              | 19.09                             | 64.50                              | <i>SiHF<sub>2</sub></i>                            | -139.51                           | 65.03                              |
| <i>Si</i> <sub>3</sub>                                    | 151.94                            | 63.98                              | <i>SiHF<sub>3</sub></i>                            | -288.52                           | 66.62                              |
| <i>Si</i> <sub>3</sub> <i>H</i> <sub>8</sub>              | 28.89                             | 81.52                              | <i>SiN</i>                                         | 115.50                            | 51.93                              |
| <i>Si</i> <sub>3</sub> <i>N</i> <sub>4</sub> ( <i>A</i> ) | -177.93                           | 26.98                              | <i>SiNH</i>                                        | 38.38                             | 51.64                              |
| <i>SiC</i>                                                | 171.94                            | 50.91                              | <i>SiNH<sub>2</sub></i>                            | 48.65                             | 58.54                              |
| <i>SiC(B)</i>                                             | -17.49                            | 3.98                               | <i>SN</i>                                          | 62.97                             | 53.02                              |
| <i>SiC</i> <sub>2</sub>                                   | 146.94                            | 56.53                              | <i>SO</i>                                          | 1.19                              | 52.99                              |
| <i>SiCl</i>                                               | 37.88                             | 56.77                              | <i>SO</i> <sub>2</sub>                             | -70.92                            | 59.27                              |
| <i>SiCl</i> <sub>2</sub>                                  | -40.28                            | 67.17                              | <i>SO</i> <sub>3</sub>                             | -94.55                            | 61.32                              |
| <i>SiCl</i> <sub>2</sub> <i>H</i> <sub>2</sub>            | -74.47                            | 68.37                              |                                                    |                                   |                                    |
| <i>SiCl</i> <sub>3</sub>                                  | -76.47                            | 75.47                              |                                                    |                                   |                                    |

## APPENDIX B. DATA BASE LISTING IN THE CHEMKIN FORMAT

Chemkin expects the thermodynamic data in a specific format, which is essentially the same as that used by the NASA Complex Chemical Equilibrium Program.<sup>13</sup> In addition to the fourteen fit coefficients, the data base also contains the species' name, its elemental composition, its electronic charge, and an indication of its phase (gas, liquid or solid). The data for each species requires four formatted 80 column card images. Table B1 provides the data format specification.

TABLE B1.  
FORMAT FOR THERMODYNAMIC DATA

| Card Number | Contents                                                                                        | Format    | Card Column |
|-------------|-------------------------------------------------------------------------------------------------|-----------|-------------|
| 1           | Species name (must start in Column 1)                                                           | 18A1      | 1 to 18     |
|             | Date (not used in the code)                                                                     | 6A1       | 19 to 24    |
|             | Atomic symbols and formula                                                                      | 4(2A1,I3) | 25 to 44    |
|             | Phase of species (S, L, or G for solid, liquid, or gas, respectively)                           | A1        | 45          |
|             | Low temperature                                                                                 | E10.0     | 46 to 55    |
|             | High temperature                                                                                | E10.0     | 56 to 65    |
|             | Common temperature (if needed)<br>(blank for default)                                           | E8.0      | 66 to 73    |
|             | Atomic symbols and formula (if needed)<br>(blank for default)                                   | 2A1,I3    | 74 to 78    |
|             | The integer "1"                                                                                 | I1        | 80          |
| 2           | Coefficients $a_1 - a_5$ in Eqs. (1-3),<br>for upper temperature interval                       | 5(E15.0)  | 1 to 75     |
|             | The integer "2"                                                                                 | I1        | 80          |
| 3           | Coefficients $a_6, a_7$ for upper temperature interval,<br>and $a_1, a_2$ , and $a_3$ for lower | 5(E15.0)  | 1 to 75     |
|             | The integer "3"                                                                                 | I1        | 80          |
| 4           | Coefficients $a_4, a_5, a_6, a_7$<br>for lower temperature interval                             | 4(E15.0)  | 1 to 60     |
|             | The integer "4"                                                                                 | I1        | 80          |

## THERMO

|        | 300.000         | 1000.000        | 5000.000        |                 |                 |         |         |  |   |
|--------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|--|---|
| AL     | 62987AL         | 1               |                 | G               | 0300.00         | 5000.00 | 0600.00 |  | 1 |
|        | 0.02559589E+02  | -0.10632239E-03 | 0.07202828E-06  | -0.02121105E-09 | 0.02289429E-13  |         |         |  | 2 |
|        | 0.03890214E+06  | 0.05234522E+02  | 0.02736825E+02  | -0.05912374E-02 | -0.04033937E-05 |         |         |  | 3 |
|        | 0.02322343E-07  | -0.01705599E-10 | 0.03886794E+06  | 0.04363879E+02  |                 |         |         |  | 4 |
| AL2H6  | 62987AL         | 2H              | 6               | G               | 0300.00         | 1500.00 | 0600.00 |  | 1 |
|        | 0.02634884E+02  | 0.02135952E+00  | 0.03154151E-05  | -0.07684674E-07 | 0.02335831E-10  |         |         |  | 2 |
|        | 0.08871346E+05  | 0.09827515E+02  | -0.06800681E+02 | 0.05080744E+00  | 0.10397471E-04  |         |         |  | 3 |
|        | -0.11195819E-06 | 0.08459155E-09  | 0.10605371E+05  | 0.05554526E+03  |                 |         |         |  | 4 |
| AL2ME6 | 62987AL         | 2C              | 6H 18           | G               | 0300.00         | 1500.00 | 0600.00 |  | 1 |
|        | 0.01773147E+03  | 0.04935747E+00  | 0.11968535E-05  | -0.16398263E-07 | 0.04890867E-10  |         |         |  | 2 |
|        | -0.03855560E+06 | -0.05053298E+03 | -0.07159750E+01 | 0.10671087E+00  | 0.02117604E-03  |         |         |  | 3 |
|        | -0.02193211E-05 | 0.16441438E-09  | -0.03515546E+06 | 0.03890762E+03  |                 |         |         |  | 4 |
| ALAS   | 62987AL         | 1AS             | 1               | G               | 0300.00         | 1500.00 | 0600.00 |  | 1 |
|        | 0.04790026E+02  | -0.01908225E-03 | -0.01983390E-05 | 0.02239358E-08  | -0.06904706E-12 |         |         |  | 2 |
|        | 0.05259290E+06  | 0.03259703E+02  | 0.05047764E+02  | -0.06419947E-02 | -0.14320714E-05 |         |         |  | 3 |
|        | 0.04754390E-07  | -0.03297621E-10 | 0.05254264E+06  | 0.01985205E+02  |                 |         |         |  | 4 |
| ALH    | 62987AL         | 1H              | 1               | G               | 0300.00         | 5000.00 | 1000.00 |  | 1 |
|        | 0.03392644E+02  | 0.12153990E-02  | -0.04676595E-05 | 0.08691624E-09  | -0.06022668E-13 |         |         |  | 2 |
|        | 0.03006845E+06  | 0.02758899E+02  | 0.03071503E+02  | 0.02165549E-01  | -0.03275638E-04 |         |         |  | 3 |
|        | 0.04136983E-07  | -0.01877120E-10 | 0.03021221E+06  | 0.04548855E+02  |                 |         |         |  | 4 |
| ALH2   | 62987AL         | 1H              | 2               | G               | 0300.00         | 1500.00 | 0600.00 |  | 1 |
|        | 0.04486543E+02  | 0.03128831E-01  | -0.01969438E-05 | -0.10160304E-08 | 0.03497468E-11  |         |         |  | 2 |
|        | 0.01960959E+06  | 0.08167897E+01  | 0.02442136E+02  | 0.09915913E-01  | 0.02471082E-05  |         |         |  | 3 |
|        | -0.02119583E-06 | 0.01710233E-09  | 0.01997587E+06  | 0.10652699E+02  |                 |         |         |  | 4 |
| ALH3   | 62987AL         | 1H              | 3               | G               | 0300.00         | 1500.00 | 0600.00 |  | 1 |
|        | 0.04186837E+02  | 0.06159249E-01  | -0.03877593E-06 | -0.02061928E-07 | 0.06600276E-11  |         |         |  | 2 |
|        | 0.07908078E+05  | 0.05134396E+01  | 0.10083231E+01  | 0.16403245E-01  | 0.01976746E-04  |         |         |  | 3 |
|        | -0.03528558E-06 | 0.02753377E-09  | 0.08484656E+05  | 0.15858377E+02  |                 |         |         |  | 4 |
| ALME   | 62987AL         | 1C              | 1H 3            | G               | 0300.00         | 1500.00 | 0600.00 |  | 1 |
|        | 0.04662737E+02  | 0.07097939E-01  | 0.02520013E-05  | -0.02114863E-07 | 0.06097489E-11  |         |         |  | 2 |
|        | 0.08203227E+05  | 0.01769244E+02  | 0.02664176E+02  | 0.13249141E-01  | 0.02525847E-04  |         |         |  | 3 |
|        | -0.02394396E-06 | 0.01761854E-09  | 0.08574173E+05  | 0.11474494E+02  |                 |         |         |  | 4 |
| ALME2  | 62987AL         | 1C              | 2H 6            | G               | 0300.00         | 1500.00 | 0600.00 |  | 1 |
|        | 0.06481282E+02  | 0.14746049E-01  | 0.05816529E-05  | -0.04621347E-07 | 0.13960405E-11  |         |         |  | 2 |
|        | 0.03745072E+05  | -0.02603325E+02 | 0.09494573E+01  | 0.03206353E+00  | 0.06134020E-04  |         |         |  | 3 |
|        | -0.06500042E-06 | 0.04911485E-09  | 0.04761408E+05  | 0.02419465E+03  |                 |         |         |  | 4 |
| ALME3  | 62987AL         | 1C              | 3H 9            | G               | 0300.00         | 1500.00 | 0600.00 |  | 1 |
|        | 0.06654948E+02  | 0.02455144E+00  | 0.11765745E-05  | -0.07815023E-07 | 0.02255622E-10  |         |         |  | 2 |
|        | -0.13409524E+05 | -0.03454481E+02 | -0.07027567E+01 | 0.04682764E+00  | 0.11499028E-04  |         |         |  | 3 |
|        | -0.09160441E-06 | 0.06687293E-09  | -0.12037989E+05 | 0.03232771E+03  |                 |         |         |  | 4 |
| AR     | 120186AR        | 1               |                 | G               | 0300.00         | 5000.00 | 1000.00 |  | 1 |
|        | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         |  | 2 |
|        | -0.07453750E+04 | 0.04366000E+02  | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  |         |         |  | 3 |
|        | 0.00000000E+00  | 0.00000000E+00  | -0.07453750E+04 | 0.04366000E+02  |                 |         |         |  | 4 |
| AR+    | 121286AR        | 1E              | -1              | G               | 0300.00         | 5000.00 | 1000.00 |  | 1 |
|        | 0.02864864E+02  | -0.12035732E-03 | -0.10651992E-07 | 0.09074839E-10  | -0.09623876E-14 |         |         |  | 2 |
|        | 0.01827230E+07  | 0.03543584E+02  | 0.02301341E+02  | 0.08035528E-02  | -0.01758805E-05 |         |         |  | 3 |
|        | -0.01781093E-08 | -0.08937268E-13 | 0.01829281E+07  | 0.06659358E+02  |                 |         |         |  | 4 |



|         |                 |                 |                 |                 |                 |         |   |
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---|
| AS      | 62987AS         | 1               | G               | 0300.00         | 1500.00         | 0600.00 | 1 |
|         | 0.02617010E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         | 2 |
|         | 0.03720454E+06  | 0.06995524E+02  | 0.02617010E+02  | 0.00000000E+00  | 0.00000000E+00  |         | 3 |
|         | 0.00000000E+00  | 0.00000000E+00  | 0.03720454E+06  | 0.06995524E+02  |                 |         | 4 |
| AS2     | 62987AS         | 2               | G               | 0300.00         | 1500.00         | 0600.00 | 1 |
|         | 0.04394201E+02  | 0.05389968E-02  | -0.02379401E-05 | -0.06541924E-09 | 0.05184186E-12  |         | 2 |
|         | 0.02235093E+06  | 0.04897918E+02  | 0.03682891E+02  | 0.03121811E-01  | -0.10740519E-05 |         | 3 |
|         | -0.05629472E-07 | 0.05178811E-10  | 0.02247355E+06  | 0.08283423E+02  |                 |         | 4 |
| AS3     | 62987AS         | 3               | G               | 0300.00         | 1500.00         | 0600.00 | 1 |
|         | 0.07404036E+02  | 0.07818425E-02  | -0.03918297E-05 | -0.05203629E-09 | 0.06291907E-12  |         | 2 |
|         | 0.03063825E+06  | -0.03417323E+02 | 0.06403142E+02  | 0.04477098E-01  | -0.01866642E-04 |         | 3 |
|         | -0.07394750E-07 | 0.07012752E-10  | 0.03080965E+06  | 0.13371355E+01  |                 |         | 4 |
| AS4     | 62987AS         | 4               | G               | 0300.00         | 1500.00         | 0600.00 | 1 |
|         | 0.09695766E+02  | 0.13062585E-02  | -0.05519564E-05 | -0.02150873E-08 | 0.14579349E-12  |         | 2 |
|         | 0.15717321E+05  | -0.16188696E+02 | 0.07853760E+02  | 0.07916509E-01  | -0.02329820E-04 |         | 3 |
|         | -0.15263119E-07 | 0.13774348E-10  | 0.16036290E+05  | -0.07409755E+02 |                 |         | 4 |
| ASALME  | 62987AS         | 1AL 1C 1H 3G    | 0300.00         | 1500.00         | 0600.00         |         | 1 |
|         | 0.07127107E+02  | 0.07357863E-01  | 0.02300796E-06  | -0.02226398E-07 | 0.06927227E-11  |         | 2 |
|         | 0.03273438E+06  | -0.01847179E+02 | 0.04053423E+02  | 0.01726125E+00  | 0.01833498E-04  |         | 3 |
|         | -0.03386952E-06 | 0.02626980E-09  | 0.03329309E+06  | 0.12996653E+02  |                 |         | 4 |
| ASALME2 | 62987AS         | 1AL 1C 2H 6G    | 0300.00         | 1500.00         | 0600.00         |         | 1 |
|         | 0.09909938E+02  | 0.14638499E-01  | 0.04118730E-05  | -0.04444657E-07 | 0.13295010E-11  |         | 2 |
|         | 0.02815111E+06  | -0.15235312E+02 | 0.04808530E+02  | 0.03067687E+00  | 0.05048000E-04  |         | 3 |
|         | -0.05908099E-06 | 0.04462290E-09  | 0.02908816E+06  | 0.09471621E+02  |                 |         | 4 |
| ASGAET  | 62987AS         | 1GA 1C 2H 5G    | 0300.00         | 1500.00         | 0600.00         |         | 1 |
|         | 0.09081073E+02  | 0.16746316E-01  | 0.12831301E-06  | -0.05590435E-07 | 0.01781314E-10  |         | 2 |
|         | 0.03807443E+06  | -0.09142782E+02 | 0.06364698E+01  | 0.04382467E+00  | 0.06144686E-04  |         | 3 |
|         | -0.09491641E-06 | 0.07374197E-09  | 0.03960893E+06  | 0.03164673E+03  |                 |         | 4 |
| ASGAET2 | 62987AS         | 1GA 1C 4H 10G   | 0300.00         | 1500.00         | 0600.00         |         | 1 |
|         | 0.10324288E+02  | 0.03073570E+00  | 0.10863354E-05  | -0.09971948E-07 | 0.02945979E-10  |         | 2 |
|         | 0.03039490E+06  | -0.13164016E+02 | -0.03539248E+01 | 0.06369772E+00  | 0.13597417E-04  |         | 3 |
|         | -0.12861423E-06 | 0.09572181E-09  | 0.03236903E+06  | 0.03865086E+03  |                 |         | 4 |
| ASGAME  | 62987AS         | 1GA 1C 1H 3G    | 0300.00         | 1500.00         | 0600.00         |         | 1 |
|         | 0.07322183E+02  | 0.06995478E-01  | 0.10693509E-06  | -0.01995283E-07 | 0.06040446E-11  |         | 2 |
|         | 0.03949448E+06  | -0.07416680E+01 | 0.04877266E+02  | 0.14825589E-01  | 0.16521240E-05  |         | 3 |
|         | -0.02712058E-06 | 0.02080195E-09  | 0.03994071E+06  | 0.11076703E+02  |                 |         | 4 |
| ASGAME2 | 62987AS         | 1GA 1C 2H 6G    | 0300.00         | 1500.00         | 0600.00         |         | 1 |
|         | 0.09352436E+02  | 0.15048197E-01  | 0.05157975E-05  | -0.04553518E-07 | 0.13487630E-11  |         | 2 |
|         | 0.03735855E+06  | -0.12181144E+02 | 0.04382076E+02  | 0.03056344E+00  | 0.05477067E-04  |         | 3 |
|         | -0.05834108E-06 | 0.04373509E-09  | 0.03827434E+06  | 0.11911109E+02  |                 |         | 4 |
| ASGAMEH | 62987AS         | 1GA 1C 1H 4G    | 0300.00         | 1500.00         | 0600.00         |         | 1 |
|         | 0.07842794E+02  | 0.09682097E-01  | 0.10603061E-06  | -0.02991402E-07 | 0.09382673E-11  |         | 2 |
|         | 0.04435297E+06  | -0.05093455E+02 | 0.03585119E+02  | 0.02336317E+00  | 0.02873356E-04  |         | 3 |
|         | -0.04737894E-06 | 0.03674461E-09  | 0.04512702E+06  | 0.15471604E+02  |                 |         | 4 |
| ASH     | 62987AS         | 1H 1            | G               | 0300.00         | 1500.00         | 0600.00 | 1 |
|         | 0.03219848E+02  | 0.10012498E-02  | -0.04874997E-08 | -0.11076533E-09 | -0.09254321E-13 |         | 2 |
|         | 0.03008175E+06  | 0.06647311E+02  | 0.03865843E+02  | -0.11575710E-02 | -0.03494371E-05 |         | 3 |
|         | 0.07079686E-07  | -0.06014027E-10 | 0.02996829E+06  | 0.03549869E+02  |                 |         | 4 |

|                 |                 |                 |                 |                 |         |         |         |   |
|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| ASH2            | 62987AS         | 1H              | 2               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.03428307E+02  | 0.03181140E-01  | 0.14604843E-06  | -0.07937145E-08 | 0.01694413E-11  |         |         |         | 2 |
| 0.02010282E+06  | 0.02904703E+02  | 0.03778945E+02  | 0.01759233E-01  | 0.08070806E-05  |         |         |         | 3 |
| 0.02358763E-07  | -0.03043521E-10 | 0.02004861E+06  | 0.12729740E+01  |                 |         |         |         | 4 |
| ASH3            | 62987AS         | 1H              | 3               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.04172022E+02  | 0.04371322E-01  | 0.02177574E-05  | -0.11832641E-08 | 0.04536373E-11  |         |         |         | 2 |
| 0.06882915E+05  | 0.02803476E+02  | 0.09446356E+01  | 0.15084686E-01  | 0.12016960E-05  |         |         |         | 3 |
| -0.03397465E-06 | 0.02767656E-09  | 0.07459168E+05  | 0.01832267E+03  |                 |         |         |         | 4 |
| ASME            | 62987AS         | 1C              | 1H 3            | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.04657260E+02  | 0.06976297E-01  | 0.02147556E-05  | -0.02101159E-07 | 0.06082149E-11  |         |         |         | 2 |
| 0.02806422E+06  | 0.03409834E+02  | 0.02625270E+02  | 0.13252423E-01  | 0.02441628E-04  |         |         |         | 3 |
| -0.02419566E-06 | 0.01786943E-09  | 0.02844080E+06  | 0.13273359E+02  |                 |         |         |         | 4 |
| ASME2           | 62987AS         | 1C              | 2H 6            | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.05981395E+02  | 0.15212837E-01  | 0.06993355E-05  | -0.04721619E-07 | 0.13699115E-11  |         |         |         | 2 |
| 0.14679847E+05  | 0.11927411E+01  | 0.13903998E+01  | 0.02923331E+00  | 0.06598870E-04  |         |         |         | 3 |
| -0.05620559E-06 | 0.04130367E-09  | 0.15533022E+05  | 0.02349980E+03  |                 |         |         |         | 4 |
| ASME3           | 62987AS         | 1C              | 3H 9            | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.06347764E+02  | 0.02466454E+00  | 0.11546286E-05  | -0.07877435E-07 | 0.02202225E-10  |         |         |         | 2 |
| -0.16173225E+04 | -0.06316786E+01 | 0.02667388E+01  | 0.04253171E+00  | 0.11651064E-04  |         |         |         | 3 |
| -0.07914706E-06 | 0.05603126E-09  | -0.04685539E+04 | 0.02904590E+03  |                 |         |         |         | 4 |
| C               | 121086C         | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.02602087E+02  | -0.01787081E-02 | 0.09087041E-06  | -0.11499333E-10 | 0.03310844E-14  |         |         |         | 2 |
| 0.08542154E+06  | 0.04195177E+02  | 0.02498584E+02  | 0.08085776E-03  | -0.02697697E-05 |         |         |         | 3 |
| 0.03040729E-08  | -0.11066518E-12 | 0.08545878E+06  | 0.04753459E+02  |                 |         |         |         | 4 |
| C(S)            | 121286C         | 1               |                 | S               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.14901664E+01  | 0.16621256E-02  | -0.06687204E-05 | 0.12908796E-09  | -0.09205334E-13 |         |         |         | 2 |
| -0.07074018E+04 | -0.08717785E+02 | -0.06705661E+01 | 0.07181499E-01  | -0.05632921E-04 |         |         |         | 3 |
| 0.02142298E-07  | -0.04168562E-11 | -0.07339498E+03 | 0.02601595E+02  |                 |         |         |         | 4 |
| C+              | 120186C         | 1E -1           |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.02511827E+02  | -0.01735978E-03 | 0.09504267E-07  | -0.02218851E-10 | 0.01862189E-14  |         |         |         | 2 |
| 0.02166772E+07  | 0.04286130E+02  | 0.02595384E+02  | -0.04068664E-02 | 0.06892366E-05  |         |         |         | 3 |
| -0.05266488E-08 | 0.15083378E-12  | 0.02166628E+07  | 0.03895729E+02  |                 |         |         |         | 4 |
| C-              | 121686C         | 1E 1            |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.02990221E+02  | -0.09184596E-02 | 0.05055560E-05  | -0.07703410E-09 | 0.03163271E-13  |         |         |         | 2 |
| 0.06983931E+06  | 0.12594533E+01  | 0.02783902E+02  | -0.01774287E-01 | 0.03696760E-04  |         |         |         | 3 |
| -0.03066693E-07 | 0.08637622E-11  | 0.06998511E+06  | 0.02726281E+02  |                 |         |         |         | 4 |
| C2              | 121286C         | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.04135978E+02  | 0.06531618E-03  | 0.01837099E-05  | -0.05295085E-09 | 0.04712137E-13  |         |         |         | 2 |
| 0.09967272E+06  | 0.07472923E+01  | 0.06996045E+02  | -0.07400601E-01 | 0.03234703E-04  |         |         |         | 3 |
| 0.04802535E-07  | -0.03295917E-10 | 0.09897487E+06  | -0.13862268E+02 |                 |         |         |         | 4 |
| C2-             | 121286C         | 2E 1            |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.03796891E+02  | 0.02530049E-02  | 0.09709118E-06  | -0.16148038E-10 | -0.03212893E-15 |         |         |         | 2 |
| 0.05207981E+06  | 0.16581468E+01  | 0.03468011E+02  | -0.02352874E-02 | 0.12439123E-05  |         |         |         | 3 |
| 0.04705960E-08  | -0.08164274E-11 | 0.05231215E+06  | 0.03886699E+02  |                 |         |         |         | 4 |
| C2F6            | 82489C          | 2F 6            |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.16020573E+02  | 0.06273007E-01  | -0.02797778E-04 | 0.05517547E-08  | -0.04004651E-12 |         |         |         | 2 |
| -0.16756543E+06 | -0.05519459E+03 | 0.03577448E+02  | 0.03913670E+00  | -0.02714862E-03 |         |         |         | 3 |
| 0.04348459E-08  | 0.04007135E-10  | -0.16421741E+06 | 0.09098384E+02  |                 |         |         |         | 4 |

|       |                 |                 |                 |                 |                 |         |         |         |   |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| C2H   | 20387C          | 2H              | 1               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.04427688E+02  | 0.02216268E-01  | -0.06048952E-05 | 0.09882517E-09  | -0.07351179E-13 |         |         | 2       |   |
|       | 0.06590415E+06  | -0.11994418E+01 | 0.03050667E+02  | 0.06051674E-01  | -0.04956634E-04 |         |         | 3       |   |
|       | 0.02804159E-07  | -0.08193332E-11 | 0.06630011E+06  | 0.05954361E+02  |                 |         |         | 4       |   |
| C2H2  | 121386C         | 2H              | 2               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.04436770E+02  | 0.05376039E-01  | -0.01912816E-04 | 0.03286379E-08  | -0.02156709E-12 |         |         | 2       |   |
|       | 0.02566766E+06  | -0.02800338E+02 | 0.02013562E+02  | 0.15190446E-01  | -0.16163189E-04 |         |         | 3       |   |
|       | 0.09078992E-07  | -0.01912746E-10 | 0.02612444E+06  | 0.08805378E+02  |                 |         |         | 4       |   |
| C2H3  | 12787C          | 2H              | 3               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.05933468E+02  | 0.04017745E-01  | -0.03966739E-05 | -0.14412666E-09 | 0.02378643E-12  |         |         | 2       |   |
|       | 0.03185434E+06  | -0.08530313E+02 | 0.02459276E+02  | 0.07371476E-01  | 0.02109872E-04  |         |         | 3       |   |
|       | -0.13216421E-08 | -0.11847838E-11 | 0.03335225E+06  | 0.11556202E+02  |                 |         |         | 4       |   |
| C2H4  | 121286C         | 2H              | 4               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.03528418E+02  | 0.11485185E-01  | -0.04418385E-04 | 0.07844600E-08  | -0.05266848E-12 |         |         | 2       |   |
|       | 0.04428288E+05  | 0.02230389E+02  | -0.08614880E+01 | 0.02796162E+00  | -0.03388677E-03 |         |         | 3       |   |
|       | 0.02785152E-06  | -0.09737879E-10 | 0.05573046E+05  | 0.02421148E+03  |                 |         |         | 4       |   |
| C2H5  | 12387C          | 2H              | 5               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.07190480E+02  | 0.06484077E-01  | -0.06428064E-05 | -0.02347879E-08 | 0.03880877E-12  |         |         | 2       |   |
|       | 0.10674549E+05  | -0.14780892E+02 | 0.02690701E+02  | 0.08719133E-01  | 0.04419838E-04  |         |         | 3       |   |
|       | 0.09338703E-08  | -0.03927773E-10 | 0.12870404E+05  | 0.12138195E+02  |                 |         |         | 4       |   |
| C2H6  | 121686C         | 2H              | 6               | G               | 0300.00         | 4000.00 | 1000.00 | 1       |   |
|       | 0.04825938E+02  | 0.13840429E-01  | -0.04557258E-04 | 0.06724967E-08  | -0.03598161E-12 |         |         | 2       |   |
|       | -0.12717793E+05 | -0.05239506E+02 | 0.14625388E+01  | 0.15494667E-01  | 0.05780507E-04  |         |         | 3       |   |
|       | -0.12578319E-07 | 0.04586267E-10  | -0.11239176E+05 | 0.14432295E+02  |                 |         |         | 4       |   |
| C2HCL | 112989C         | 2H              | 1CL             | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|       | 0.06295372E+02  | 0.03883113E-01  | -0.15060494E-05 | 0.02700003E-08  | -0.01830213E-12 |         |         | 2       |   |
|       | 0.02357278E+06  | -0.08137063E+02 | 0.03618443E+02  | 0.13319791E-01  | -0.13218222E-04 |         |         | 3       |   |
|       | 0.06092023E-07  | -0.08879026E-11 | 0.02415385E+06  | 0.05050645E+02  |                 |         |         | 4       |   |
| C2N   | 121286C         | 2N              | 1               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.06151561E+02  | 0.15116498E-02  | -0.06629362E-05 | 0.12861485E-09  | -0.09160830E-13 |         |         | 2       |   |
|       | 0.06484318E+06  | -0.08177850E+02 | 0.03498544E+02  | 0.08554433E-01  | -0.06288697E-04 |         |         | 3       |   |
|       | 0.08638478E-08  | 0.04915996E-11  | 0.06556611E+06  | 0.05548374E+02  |                 |         |         | 4       |   |
| C2N2  | 121286C         | 2N              | 2               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.06548002E+02  | 0.03984707E-01  | -0.16342164E-05 | 0.03038596E-08  | -0.02111069E-12 |         |         | 2       |   |
|       | 0.03490716E+06  | -0.09735790E+02 | 0.04265459E+02  | 0.11922569E-01  | -0.13420142E-04 |         |         | 3       |   |
|       | 0.09192297E-07  | -0.02778941E-10 | 0.03547887E+06  | 0.01713212E+02  |                 |         |         | 4       |   |
| C2O   | 121286C         | 2O              | 1               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.04849809E+02  | 0.02947585E-01  | -0.10907286E-05 | 0.01792562E-08  | -0.11157585E-13 |         |         | 2       |   |
|       | 0.03282055E+06  | -0.06453225E+01 | 0.03368850E+02  | 0.08241803E-01  | -0.08765145E-04 |         |         | 3       |   |
|       | 0.05569262E-07  | -0.15400086E-11 | 0.03317081E+06  | 0.06713314E+02  |                 |         |         | 4       |   |
| C3    | 121286C         | 3               |                 | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.03803709E+02  | 0.02253566E-01  | -0.07704534E-05 | 0.13162939E-09  | -0.08694264E-13 |         |         | 2       |   |
|       | 0.09736135E+06  | 0.06128062E+02  | 0.04345527E+02  | 0.12644661E-02  | -0.04652557E-04 |         |         | 3       |   |
|       | 0.08695855E-07  | -0.04243535E-10 | 0.09731403E+06  | 0.03519437E+02  |                 |         |         | 4       |   |
| C3H2  | 121686C         | 3H              | 2               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.06530853E+02  | 0.05870316E-01  | -0.01720776E-04 | 0.02127498E-08  | -0.08291910E-13 |         |         | 2       |   |
|       | 0.05115213E+06  | -0.11227278E+02 | 0.02691077E+02  | 0.14803664E-01  | -0.03250551E-04 |         |         | 3       |   |
|       | -0.08644363E-07 | 0.05284877E-10  | 0.05219072E+06  | 0.08757391E+02  |                 |         |         | 4       |   |

|                                                                             |         |    |   |   |         |         |         |   |
|-----------------------------------------------------------------------------|---------|----|---|---|---------|---------|---------|---|
| C3H4                                                                        | 40687C  | 3H | 4 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.05729144E+02 0.12368045E-01-0.04805626E-04 0.08601364E-08-0.05812802E-12  |         |    |   |   |         |         |         |   |
| 0.02012984E+06-0.09448668E+02-0.02131968E+01 0.03358713E+00-0.03804870E-03  |         |    |   |   |         |         |         |   |
| 0.02745838E-06-0.08690044E-10 0.02162048E+06 0.02029392E+03                 |         |    |   |   |         |         |         |   |
| C3H4C                                                                       | 121686C | 3H | 4 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.06699993E+02 0.10357372E-01-0.03455116E-04 0.05065295E-08-0.02668227E-12  |         |    |   |   |         |         |         |   |
| 0.03019905E+06-0.13391933E+02-0.02462104E+00 0.02319721E+00-0.01847435E-04  |         |    |   |   |         |         |         |   |
| -0.15927594E-07 0.08684615E-10 0.03233413E+06 0.02271659E+03                |         |    |   |   |         |         |         |   |
| C3H4P                                                                       | 40687C  | 3H | 4 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.05511034E+02 0.12469562E-01-0.04814164E-04 0.08573770E-08-0.05771561E-12  |         |    |   |   |         |         |         |   |
| 0.01961967E+06-0.10794748E+02 0.06271447E+01 0.03116179E+00-0.03747663E-03  |         |    |   |   |         |         |         |   |
| 0.02964117E-06-0.09987381E-10 0.02083492E+06 0.13468796E+02                 |         |    |   |   |         |         |         |   |
| C3H6                                                                        | 120186C | 3H | 6 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.06732257E+02 0.14908336E-01-0.04949899E-04 0.07212022E-08-0.03766204E-12  |         |    |   |   |         |         |         |   |
| -0.09235703E+04-0.13313348E+02 0.14933071E+01 0.02092517E+00 0.04486794E-04 |         |    |   |   |         |         |         |   |
| -0.16689121E-07 0.07158146E-10 0.10748264E+04 0.16145340E+02                |         |    |   |   |         |         |         |   |
| C3H8                                                                        | 120186C | 3H | 8 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.07525217E+02 0.01889034E+00-0.06283924E-04 0.09179373E-08-0.04812410E-12  |         |    |   |   |         |         |         |   |
| -0.16464548E+05-0.01784390E+03 0.08969208E+01 0.02668986E+00 0.05431425E-04 |         |    |   |   |         |         |         |   |
| -0.02126000E-06 0.09243330E-10-0.13954918E+05 0.01935533E+03                |         |    |   |   |         |         |         |   |
| C3O2                                                                        | 121286C | 3O | 2 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.08098897E+02 0.05560039E-01-0.02312264E-04 0.04340709E-08-0.03036387E-12  |         |    |   |   |         |         |         |   |
| -0.14214353E+05-0.15219745E+02 0.04018127E+02 0.01836660E+00-0.01907148E-03 |         |    |   |   |         |         |         |   |
| 0.11855871E-07-0.03418747E-10-0.13128236E+05 0.05582083E+02                 |         |    |   |   |         |         |         |   |
| C4                                                                          | 121286C | 4  |   | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.06500180E+02 0.04228632E-01-0.01790717E-04 0.03404812E-08-0.02403978E-12  |         |    |   |   |         |         |         |   |
| 0.11434008E+06-0.11488894E+02 0.02343028E+02 0.16429811E-01-0.15279858E-04  |         |    |   |   |         |         |         |   |
| 0.07343826E-07-0.15822743E-11 0.11545384E+06 0.09826204E+02                 |         |    |   |   |         |         |         |   |
| C4H                                                                         | 121686C | 4H | 1 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.06242882E+02 0.06193682E-01-0.02085931E-04 0.03082203E-08-0.16364826E-13  |         |    |   |   |         |         |         |   |
| 0.07568019E+06-0.07210806E+02 0.05023247E+02 0.07092375E-01-0.06073762E-07  |         |    |   |   |         |         |         |   |
| -0.02275752E-07 0.08086994E-11 0.07623812E+06-0.06942594E+00                |         |    |   |   |         |         |         |   |
| C4H2                                                                        | 121686C | 4H | 2 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.09031407E+02 0.06047252E-01-0.01948788E-04 0.02754863E-08-0.13856080E-13  |         |    |   |   |         |         |         |   |
| 0.05294735E+06-0.02385067E+03 0.04005191E+02 0.01981000E+00-0.09865877E-04  |         |    |   |   |         |         |         |   |
| -0.06635158E-07 0.06077413E-10 0.05424065E+06 0.01845736E+02                |         |    |   |   |         |         |         |   |
| C4H6                                                                        | 120186C | 4H | 6 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.08046583E+02 0.16485251E-01-0.05522227E-04 0.08123593E-08-0.04295078E-12  |         |    |   |   |         |         |         |   |
| 0.13701305E+05-0.01800457E+03 0.03197108E+02 0.02025591E+00 0.06510192E-04  |         |    |   |   |         |         |         |   |
| -0.16584423E-07 0.06400282E-10 0.15715203E+05 0.09895660E+02                |         |    |   |   |         |         |         |   |
| C4H8                                                                        | 120386C | 4H | 8 | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.02053584E+02 0.03435050E+00-0.15883196E-04 0.03308966E-07-0.02536104E-11  |         |    |   |   |         |         |         |   |
| -0.02139723E+05 0.15543201E+02 0.11811380E+01 0.03085338E+00 0.05086524E-04 |         |    |   |   |         |         |         |   |
| -0.02465488E-06 0.11110192E-10-0.01790400E+05 0.02106247E+03                |         |    |   |   |         |         |         |   |
| C5                                                                          | 121286C | 5  |   | G | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.08078081E+02 0.05743464E-01-0.02436405E-04 0.04638916E-08-0.03278909E-12  |         |    |   |   |         |         |         |   |
| 0.11470216E+06-0.01953023E+03 0.02115273E+02 0.02326331E+00-0.02109499E-03  |         |    |   |   |         |         |         |   |
| 0.09072734E-07-0.15400926E-11 0.11627381E+06 0.10976027E+02                 |         |    |   |   |         |         |         |   |

|       |                 |                 |                 |                 |                 |         |         |   |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---|
| C5H   | 20387C          | 5H              | 1               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.08695749E+02  | 0.06054301E-01  | -0.02016010E-04 | 0.02892892E-08  | -0.14700996E-13 |         |         | 2 |
|       | 0.09031069E+06  | -0.02101594E+03 | 0.16348248E+01  | 0.02509538E+00  | -0.12066364E-04 |         |         | 3 |
|       | -0.10465110E-07 | 0.08809988E-10  | 0.09212488E+06  | 0.15121937E+02  |                 |         |         | 4 |
| C5H12 | 20387C          | 5H              | 12              | G               | 0300.00         | 4000.00 | 1000.00 | 1 |
|       | 0.16677979E+02  | 0.02114483E+00  | -0.03533321E-04 | -0.05742202E-08 | 0.15159483E-12  |         |         | 2 |
|       | -0.02553670E+06 | -0.06372940E+03 | 0.01877907E+02  | 0.04121645E+00  | 0.12532337E-04  |         |         | 3 |
|       | -0.03701536E-06 | 0.15255685E-10  | -0.02003815E+06 | 0.01877256E+03  |                 |         |         | 4 |
| C5H2  | 20587C          | 5H              | 2               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.11329175E+02  | 0.07424056E-01  | -0.02628188E-04 | 0.04082541E-08  | -0.02301332E-12 |         |         | 2 |
|       | 0.07878706E+06  | -0.03617117E+03 | 0.03062321E+02  | 0.02709998E+00  | -0.10091697E-04 |         |         | 3 |
|       | -0.12727451E-07 | 0.09167219E-10  | 0.08114969E+06  | 0.07071078E+02  |                 |         |         | 4 |
| C5H3  | 20387C          | 5H              | 3               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.10787622E+02  | 0.09539619E-01  | -0.03206744E-04 | 0.04733323E-08  | -0.02512135E-12 |         |         | 2 |
|       | 0.06392904E+06  | -0.03005444E+03 | 0.04328720E+02  | 0.02352480E+00  | -0.05856723E-04 |         |         | 3 |
|       | -0.12154494E-07 | 0.07726478E-10  | 0.06588531E+06  | 0.04173258E+02  |                 |         |         | 4 |
| C5H6  | 20387C          | 5H              | 6               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.09689815E+02  | 0.01838262E+00  | -0.06264884E-04 | 0.09393377E-08  | -0.05087708E-12 |         |         | 2 |
|       | 0.11021242E+05  | -0.03122908E+03 | -0.03196739E+02 | 0.04081361E+00  | 0.06816505E-05  |         |         | 3 |
|       | -0.03137459E-06 | 0.15772230E-10  | 0.15290676E+05  | 0.03869938E+03  |                 |         |         | 4 |
| C6H   | 121686C         | 6H              | 1               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.11587352E+02  | 0.07295362E-01  | -0.02466008E-04 | 0.03407045E-08  | -0.14981855E-13 |         |         | 2 |
|       | 0.10314481E+06  | -0.03172578E+03 | 0.04769848E+02  | 0.02457279E+00  | -0.07561252E-04 |         |         | 3 |
|       | -0.14806908E-07 | 0.09768053E-10  | 0.10485231E+06  | 0.03241530E+02  |                 |         |         | 4 |
| C6H10 | 20387C          | 6H              | 10              | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.15927771E+02  | 0.02374412E+00  | -0.06908672E-04 | 0.08109777E-08  | -0.02683122E-12 |         |         | 2 |
|       | -0.08642656E+05 | -0.06525186E+03 | -0.13942280E+01 | 0.04720693E+00  | 0.11960419E-04  |         |         | 3 |
|       | -0.04162895E-06 | 0.01740335E-09  | -0.02217790E+05 | 0.03129603E+03  |                 |         |         | 4 |
| C6H14 | 20387C          | 6H              | 14              | G               | 0300.00         | 4000.00 | 1000.00 | 1 |
|       | 0.02280471E+03  | 0.02097989E+00  | -0.03530674E-04 | -0.05466245E-08 | 0.14789499E-12  |         |         | 2 |
|       | -0.03073756E+06 | -0.09583162E+03 | 0.01836174E+02  | 0.05098461E+00  | 0.12595857E-04  |         |         | 3 |
|       | -0.04428362E-06 | 0.01872237E-09  | -0.02292749E+06 | 0.02088145E+03  |                 |         |         | 4 |
| C6H2  | 121686C         | 6H              | 2               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.12756519E+02  | 0.08034381E-01  | -0.02618215E-04 | 0.03725060E-08  | -0.01878850E-12 |         |         | 2 |
|       | 0.08075469E+06  | -0.04041262E+03 | 0.05751085E+02  | 0.02636719E+00  | -0.11667596E-04 |         |         | 3 |
|       | -0.10714498E-07 | 0.08790297E-10  | 0.08262012E+06  | -0.04335532E+02 |                 |         |         | 4 |
| C6H3  | 20387C          | 6H              | 3               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.12761181E+02  | 0.10385573E-01  | -0.03479192E-04 | 0.05109733E-08  | -0.02690965E-12 |         |         | 2 |
|       | 0.07477706E+06  | -0.03891745E+03 | 0.05007089E+02  | 0.02692851E+00  | -0.05919865E-04 |         |         | 3 |
|       | -0.15272335E-07 | 0.09408310E-10  | 0.07713200E+06  | 0.02225621E+02  |                 |         |         | 4 |
| C6H4  | 20387C          | 6H              | 4               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|       | 0.10062741E+02  | 0.01690304E+00  | -0.06473045E-04 | 0.11240806E-08  | -0.07307566E-12 |         |         | 2 |
|       | 0.05645373E+06  | -0.02969310E+03 | -0.13004846E+01 | 0.03866476E+00  | -0.03643944E-04 |         |         | 3 |
|       | -0.02668580E-06 | 0.14509357E-10  | 0.06002907E+06  | 0.03124939E+03  |                 |         |         | 4 |
| C6H5  | 82489C          | 6H              | 5               | G               | 0300.00         | 4000.00 | 1000.00 | 1 |
|       | 0.15775887E+02  | 0.09651109E-01  | -0.09429416E-05 | -0.05469111E-08 | 0.10265216E-12  |         |         | 2 |
|       | 0.03302698E+06  | -0.06176280E+03 | 0.11435567E+00  | 0.03627324E+00  | 0.11582856E-05  |         |         | 3 |
|       | -0.02196964E-06 | 0.08463556E-10  | 0.03836054E+06  | 0.02380117E+03  |                 |         |         | 4 |

|                 |                 |                 |                 |                 |         |         |         |         |
|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---------|
| C6H5(L)         | 82489C          | 6H              | 5               | G               | 0300.00 | 4000.00 | 1000.00 | 1       |
| 0.01721540E+03  | 0.08621068E-01  | -0.08221340E-05 | -0.04752164E-08 | 0.08844086E-12  |         |         |         | 2       |
| 0.06385819E+06  | -0.06139128E+03 | 0.04854268E+02  | 0.03031659E+00  | 0.01742892E-05  |         |         |         | 3       |
| -0.01811010E-06 | 0.07392511E-10  | 0.06798733E+06  | 0.05854934E+02  |                 |         |         |         | 4       |
| C6H5O           | 82489C          | 6H              | 50              | 1               | G       | 0300.00 | 4000.00 | 1000.00 |
| 0.01822638E+03  | 0.10039851E-01  | -0.09915668E-05 | -0.05672804E-08 | 0.10683716E-12  |         |         |         | 2       |
| -0.02620846E+05 | -0.07361390E+03 | 0.11074965E+01  | 0.03956945E+00  | 0.08497295E-05  |         |         |         | 3       |
| -0.02436311E-06 | 0.09650659E-10  | 0.03159672E+05  | 0.01973496E+03  |                 |         |         |         | 4       |
| C6H5OH          | 82489C          | 6H              | 60              | 1               | G       | 0300.00 | 4000.00 | 1000.00 |
| 0.01821632E+03  | 0.11424269E-01  | -0.10966843E-05 | -0.06427442E-08 | 0.11988930E-12  |         |         |         | 2       |
| -0.02053664E+06 | -0.07304233E+03 | 0.13914556E+01  | 0.03931957E+00  | 0.01777096E-04  |         |         |         | 3       |
| -0.02277673E-06 | 0.08309659E-10  | -0.14721809E+05 | 0.01917813E+03  |                 |         |         |         | 4       |
| C6H6            | 20387C          | 6H              | 6               | G               | 0300.00 | 5000.00 | 1000.00 | 1       |
| 0.12910740E+02  | 0.01723296E+00  | -0.05024210E-04 | 0.05893497E-08  | -0.01947521E-12 |         |         |         | 2       |
| 0.03664511E+05  | -0.05002699E+03 | -0.03138012E+02 | 0.04723103E+00  | -0.02962207E-04 |         |         |         | 3       |
| -0.03262819E-06 | 0.01718691E-09  | 0.08890031E+05  | 0.03657573E+03  |                 |         |         |         | 4       |
| C6H7            | 82489C          | 6H              | 7               | G               | 0300.00 | 4000.00 | 1000.00 | 1       |
| 0.01755221E+03  | 0.12270795E-01  | -0.11857424E-05 | -0.06959661E-08 | 0.13013259E-12  |         |         |         | 2       |
| 0.16245813E+05  | -0.07166588E+03 | 0.04639166E+01  | 0.03975928E+00  | 0.02529095E-04  |         |         |         | 3       |
| -0.02223792E-06 | 0.07557053E-10  | 0.02225169E+06  | 0.02235387E+03  |                 |         |         |         | 4       |
| C8H             | 121686C         | 8H              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1       |
| 0.14749907E+02  | 0.09931501E-01  | -0.03374841E-04 | 0.04687592E-08  | -0.02073536E-12 |         |         |         | 2       |
| 0.13994481E+06  | -0.04892689E+03 | 0.04489507E+02  | 0.03521521E+00  | -0.10193898E-04 |         |         |         | 3       |
| -0.02197024E-06 | 0.14214164E-10  | 0.14259919E+06  | 0.03996225E+02  |                 |         |         |         | 4       |
| C8H2            | 121686C         | 8H              | 2               | G               | 0300.00 | 5000.00 | 1000.00 | 1       |
| 0.15680213E+02  | 0.11154614E-01  | -0.03724372E-04 | 0.05197891E-08  | -0.02375550E-12 |         |         |         | 2       |
| 0.10811225E+06  | -0.05571437E+03 | 0.04630427E+02  | 0.03937080E+00  | -0.11480348E-04 |         |         |         | 3       |
| -0.02562213E-06 | 0.16707913E-10  | 0.11082850E+06  | 0.08077425E+01  |                 |         |         |         | 4       |
| CCL             | 112989C         | 1CL             | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1       |
| 0.04072804E+02  | 0.05508787E-02  | -0.02319334E-05 | 0.04669038E-09  | -0.03236856E-13 |         |         |         | 2       |
| 0.05909198E+06  | 0.03481073E+02  | 0.03188782E+02  | 0.02965197E-01  | -0.02305370E-04 |         |         |         | 3       |
| 0.04866913E-08  | 0.09990141E-12  | 0.05932937E+06  | 0.08037628E+02  |                 |         |         |         | 4       |
| CCL2            | 112989C         | 1CL             | 2               | G               | 0300.00 | 5000.00 | 1000.00 | 1       |
| 0.03501741E+02  | 0.05749397E-01  | -0.02589721E-04 | 0.04783950E-08  | -0.03188271E-12 |         |         |         | 2       |
| 0.02763633E+06  | 0.10829469E+02  | 0.02651916E+02  | 0.15169552E-01  | -0.02230162E-03 |         |         |         | 3       |
| 0.15041039E-07  | -0.03452951E-10 | 0.02739027E+06  | 0.13136703E+02  |                 |         |         |         | 4       |
| CCL3            | 112989C         | 1CL             | 3               | G               | 0300.00 | 5000.00 | 1000.00 | 1       |
| 0.08639372E+02  | 0.15880909E-02  | -0.07176410E-05 | 0.14271238E-09  | -0.10407368E-13 |         |         |         | 2       |
| 0.06701065E+05  | -0.14518221E+02 | 0.04866162E+02  | 0.11903691E-01  | -0.07849049E-04 |         |         |         | 3       |
| -0.14484371E-08 | 0.02169760E-10  | 0.07655364E+05  | 0.04781636E+02  |                 |         |         |         | 4       |
| CCL4            | 112989C         | 1CL             | 4               | G               | 0300.00 | 5000.00 | 1000.00 | 1       |
| 0.11369968E+02  | 0.01933276E-01  | -0.08832003E-05 | 0.01770067E-08  | -0.12982896E-13 |         |         |         | 2       |
| -0.15283466E+05 | -0.02874324E+03 | 0.06286815E+02  | 0.15997799E-01  | -0.10203526E-04 |         |         |         | 3       |
| -0.03043311E-07 | 0.03546287E-10  | -0.14032573E+05 | -0.02850812E+02 |                 |         |         |         | 4       |
| CH              | 121286C         | 1H              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1       |
| 0.02196223E+02  | 0.02340381E-01  | -0.07058201E-05 | 0.09007582E-09  | -0.03855040E-13 |         |         |         | 2       |
| 0.07086723E+06  | 0.09178373E+02  | 0.03200202E+02  | 0.02072875E-01  | -0.05134431E-04 |         |         |         | 3       |
| 0.05733890E-07  | -0.01955533E-10 | 0.07045259E+06  | 0.03331587E+02  |                 |         |         |         | 4       |



|            |                 |                 |                 |                 |                 |         |         |         |   |
|------------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| CH+        | 121286C         | 1H              | 1E              | -1              | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.02753358E+02  | 0.15528998E-02  | -0.05368453E-05 | 0.08921772E-09  | -0.05416801E-13 |         |         |         | 2 |
|            | 0.01948467E+07  | 0.04654892E+02  | 0.03327207E+02  | 0.13470505E-02  | -0.03895861E-04 |         |         |         | 3 |
|            | 0.05129390E-07  | -0.02054575E-10 | 0.01946452E+07  | 0.14084738E+01  |                 |         |         |         | 4 |
| CH2        | 120186C         | 1H              | 2               |                 | G               | 0250.00 | 4000.00 | 1000.00 | 1 |
|            | 0.03636407E+02  | 0.01933056E-01  | -0.01687016E-05 | -0.10098994E-09 | 0.01808255E-12  |         |         |         | 2 |
|            | 0.04534134E+06  | 0.02156560E+02  | 0.03762237E+02  | 0.11598191E-02  | 0.02489585E-05  |         |         |         | 3 |
|            | 0.08800836E-08  | -0.07332435E-11 | 0.04536790E+06  | 0.01712577E+02  |                 |         |         |         | 4 |
| CH2(S)     | 31287C          | 1H              | 2               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.03552888E+02  | 0.02066788E-01  | -0.01914116E-05 | -0.11046733E-09 | 0.02021349E-12  |         |         |         | 2 |
|            | 0.04984975E+06  | 0.01686570E+02  | 0.03971265E+02  | -0.01699088E-02 | 0.10253689E-05  |         |         |         | 3 |
|            | 0.02492550E-07  | -0.01981266E-10 | 0.04989367E+06  | 0.05753207E+00  |                 |         |         |         | 4 |
| CH2CHCCH   | 82489C          | 4H              | 4               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.10697773E+02  | 0.06982014E-01  | -0.06567747E-05 | -0.03884517E-08 | 0.07200946E-12  |         |         |         | 2 |
|            | 0.03034803E+06  | -0.03128430E+03 | 0.03233893E+02  | 0.01865634E+00  | 0.12703205E-05  |         |         |         | 3 |
|            | -0.09410096E-07 | 0.02956110E-10  | 0.03301097E+06  | 0.09922676E+02  |                 |         |         |         | 4 |
| CH2CHCCH2  | 82489C          | 4H              | 5               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.11997762E+02  | 0.07990580E-01  | -0.08098172E-05 | -0.04568733E-08 | 0.08636911E-12  |         |         |         | 2 |
|            | 0.03228493E+06  | -0.03528494E+03 | 0.03879443E+02  | 0.01997663E+00  | 0.01872777E-04  |         |         |         | 3 |
|            | -0.09306953E-07 | 0.02386116E-10  | 0.03526859E+06  | 0.09842152E+02  |                 |         |         |         | 4 |
| CH2CHCH2   | 82489C          | 3H              | 5               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.09651539E+02  | 0.08075596E-01  | -0.07965424E-05 | -0.04650696E-08 | 0.08603281E-12  |         |         |         | 2 |
|            | 0.15300955E+05  | -0.02686773E+03 | 0.02276486E+02  | 0.01985564E+00  | 0.11238421E-05  |         |         |         | 3 |
|            | -0.10145757E-07 | 0.03441342E-10  | 0.01789496E+06  | 0.13725151E+02  |                 |         |         |         | 4 |
| CH2CHCHCH  | 82489C          | 4H              | 5               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.12865971E+02  | 0.07943369E-01  | -0.08626466E-05 | -0.04655635E-08 | 0.08951131E-12  |         |         |         | 2 |
|            | 0.03783552E+06  | -0.04182502E+03 | 0.02995240E+02  | 0.02288456E+00  | 0.01975471E-04  |         |         |         | 3 |
|            | -0.11482454E-07 | 0.03197823E-10  | 0.04142218E+06  | 0.12894539E+02  |                 |         |         |         | 4 |
| CH2CHCHCH2 | 120189C         | 4H              | 6               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.12544366E+02  | 0.09596525E-01  | -0.09187012E-05 | -0.05429640E-08 | 0.10053636E-12  |         |         |         | 2 |
|            | 0.08597330E+05  | -0.04217450E+03 | 0.01931624E+02  | 0.02479030E+00  | 0.03018071E-04  |         |         |         | 3 |
|            | -0.11546856E-07 | 0.02586623E-10  | 0.12554682E+05  | 0.01701999E+03  |                 |         |         |         | 4 |
| CH2CL2     | 112989C         | 1H              | 2CL             | 2               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.05917327E+02  | 0.06762395E-01  | -0.02676163E-04 | 0.04856687E-08  | -0.03316973E-12 |         |         |         | 2 |
|            | -0.13859256E+05 | -0.03877739E+02 | 0.14232844E+01  | 0.02116658E+00  | -0.02178088E-03 |         |         |         | 3 |
|            | 0.13458726E-07  | -0.03811649E-10 | -0.12686636E+05 | 0.01893445E+03  |                 |         |         |         | 4 |
| CH2CO      | 121686C         | 2H              | 20              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.06038817E+02  | 0.05804840E-01  | -0.01920953E-04 | 0.02794484E-08  | -0.14588676E-13 |         |         |         | 2 |
|            | -0.08583402E+05 | -0.07657581E+02 | 0.02974970E+02  | 0.12118712E-01  | -0.02345045E-04 |         |         |         | 3 |
|            | -0.06466685E-07 | 0.03905649E-10  | -0.07632636E+05 | 0.08673553E+02  |                 |         |         |         | 4 |
| CH2F2      | 82489C          | 1H              | 2F              | 2               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.04730052E+02  | 0.07997300E-01  | -0.03186045E-04 | 0.05801159E-08  | -0.03967925E-12 |         |         |         | 2 |
|            | -0.05637288E+06 | -0.04954843E+01 | 0.03669433E+01  | 0.02168917E+00  | -0.02441912E-03 |         |         |         | 3 |
|            | 0.01942310E-06  | -0.06978343E-10 | -0.05510102E+06 | 0.02202214E+03  |                 |         |         |         | 4 |
| CH2HCO     | 120186C         | 1H              | 3C              | 2               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.05975670E+02  | 0.08130591E-01  | -0.02743624E-04 | 0.04070304E-08  | -0.02176017E-12 |         |         |         | 2 |
|            | 0.04903218E+04  | -0.05045251E+02 | 0.03409062E+02  | 0.10738574E-01  | 0.01891492E-04  |         |         |         | 3 |
|            | -0.07158583E-07 | 0.02867385E-10  | 0.15214766E+04  | 0.09558290E+02  |                 |         |         |         | 4 |

|           |                 |                 |                 |                 |                 |         |         |         |   |
|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| CH2O      | 121286C         | 1H              | 20              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.02995606E+02  | 0.06681321E-01  | -0.02628954E-04 | 0.04737153E-08  | -0.03212517E-12 |         |         |         | 2 |
|           | -0.15320369E+05 | 0.06912572E+02  | 0.16527311E+01  | 0.12631439E-01  | -0.01888168E-03 |         |         |         | 3 |
|           | 0.02050031E-06  | -0.08413237E-10 | -0.14865404E+05 | 0.13784820E+02  |                 |         |         |         | 4 |
| CH2OH     | 120186H         | 3C              | 10              | 1               | G               | 0250.00 | 4000.00 | 1000.00 | 1 |
|           | 0.06327520E+02  | 0.03608270E-01  | -0.03201547E-05 | -0.01938750E-08 | 0.03509704E-12  |         |         |         | 2 |
|           | -0.04474509E+05 | -0.08329365E+02 | 0.02862628E+02  | 0.10015273E-01  | -0.05285435E-05 |         |         |         | 3 |
|           | -0.05138539E-07 | 0.02246041E-10  | -0.03349678E+05 | 0.10397938E+02  |                 |         |         |         | 4 |
| CH3       | 121286C         | 1H              | 3               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.02844051E+02  | 0.06137974E-01  | -0.02230345E-04 | 0.03785161E-08  | -0.02452159E-12 |         |         |         | 2 |
|           | 0.16437809E+05  | 0.05452697E+02  | 0.02430442E+02  | 0.11124099E-01  | -0.01680220E-03 |         |         |         | 3 |
|           | 0.16218288E-07  | -0.05864952E-10 | 0.16423781E+05  | 0.06789794E+02  |                 |         |         |         | 4 |
| CH3CC     | 82489C          | 3H              | 3               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.07640221E+02  | 0.05233556E-01  | -0.05053635E-05 | -0.02919772E-08 | 0.05445700E-12  |         |         |         | 2 |
|           | 0.05909763E+06  | -0.16295735E+02 | 0.03798751E+02  | 0.08749062E-01  | 0.02523014E-04  |         |         |         | 3 |
|           | -0.15293730E-08 | -0.14105619E-11 | 0.06077425E+06  | 0.05989223E+02  |                 |         |         |         | 4 |
| CH3CCCH2  | 82489C          | 4H              | 5               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.11565059E+02  | 0.08030297E-01  | -0.07649450E-05 | -0.04476533E-08 | 0.08313260E-12  |         |         |         | 2 |
|           | 0.03256813E+06  | -0.03014066E+03 | 0.05068450E+02  | 0.15717475E-01  | 0.02968975E-04  |         |         |         | 3 |
|           | -0.04990586E-07 | -0.02984224E-11 | 0.03518855E+06  | 0.06791893E+02  |                 |         |         |         | 4 |
| CH3CCCH3  | 120189C         | 4H              | 6               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.11336582E+02  | 0.10057637E-01  | -0.09511323E-05 | -0.05660496E-08 | 0.10494509E-12  |         |         |         | 2 |
|           | 0.15476594E+05  | -0.03350866E+03 | 0.04077105E+02  | 0.01703158E+00  | 0.04707490E-04  |         |         |         | 3 |
|           | -0.03767239E-07 | -0.02066962E-10 | 0.01859756E+06  | 0.08444801E+02  |                 |         |         |         | 4 |
| CH3CCH2   | 82489C          | 3H              | 5               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.09101018E+02  | 0.07964167E-01  | -0.07884945E-05 | -0.04562036E-08 | 0.08529212E-12  |         |         |         | 2 |
|           | 0.02670680E+06  | -0.02150559E+03 | 0.03385811E+02  | 0.14045337E-01  | 0.03204127E-04  |         |         |         | 3 |
|           | -0.03824120E-07 | -0.09053742E-11 | 0.02909066E+06  | 0.11266487E+02  |                 |         |         |         | 4 |
| CH3CH2CCH | 120189C         | 4H              | 6               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.12006946E+02  | 0.09576069E-01  | -0.08995018E-05 | -0.05369808E-08 | 0.09934174E-12  |         |         |         | 2 |
|           | 0.01729419E+06  | -0.03802692E+03 | 0.03726043E+02  | 0.02053492E+00  | 0.03021439E-04  |         |         |         | 3 |
|           | -0.08131812E-07 | 0.10952799E-11  | 0.02048821E+06  | 0.08538826E+02  |                 |         |         |         | 4 |
| CH3CHCH   | 82489C          | 3H              | 5               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.09209764E+02  | 0.07871412E-01  | -0.07724522E-05 | -0.04497357E-08 | 0.08377272E-12  |         |         |         | 2 |
|           | 0.02853967E+06  | -0.02232369E+03 | 0.03161863E+02  | 0.15180997E-01  | 0.02722659E-04  |         |         |         | 3 |
|           | -0.05177112E-07 | 0.05435286E-12  | 0.03095547E+06  | 0.11979733E+02  |                 |         |         |         | 4 |
| CH3CL     | 112989C         | 1H              | 3CL             | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.03633875E+02  | 0.08664625E-01  | -0.03343871E-04 | 0.05950130E-08  | -0.04001401E-12 |         |         |         | 2 |
|           | -0.11776588E+05 | 0.04430651E+02  | 0.04621901E+01  | 0.02068247E+00  | -0.02553133E-03 |         |         |         | 3 |
|           | 0.02160310E-06  | -0.07706816E-10 | -0.10936672E+05 | 0.02032976E+03  |                 |         |         |         | 4 |
| CH3CO     | 120186C         | 2H              | 30              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.05612279E+02  | 0.08449886E-01  | -0.02854147E-04 | 0.04238376E-08  | -0.02268403E-12 |         |         |         | 2 |
|           | -0.05187863E+05 | -0.03274949E+02 | 0.03125278E+02  | 0.09778220E-01  | 0.04521448E-04  |         |         |         | 3 |
|           | -0.09009462E-07 | 0.03193717E-10  | -0.04108507E+05 | 0.11228854E+02  |                 |         |         |         | 4 |
| CH3F      | 82489C          | 1H              | 3F              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.03014978E+02  | 0.09314397E-01  | -0.03611697E-04 | 0.06443728E-08  | -0.04339594E-12 |         |         |         | 2 |
|           | -0.02977838E+06 | 0.06323815E+02  | 0.02600910E+01  | 0.02000787E+00  | -0.02662584E-03 |         |         |         | 3 |
|           | 0.02561176E-06  | -0.09935237E-10 | -0.02896232E+06 | 0.02031799E+03  |                 |         |         |         | 4 |



|                 |                 |                 |                 |                 |    |         |         |         |   |
|-----------------|-----------------|-----------------|-----------------|-----------------|----|---------|---------|---------|---|
| CH3HCO          | 120186C         | 20              | 1H              | 4               | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.05868650E+02  | 0.10794241E-01  | -0.03645530E-04 | 0.05412912E-08  | -0.02896844E-12 |    |         |         |         | 2 |
| -0.02264568E+06 | -0.06012946E+02 | 0.02505695E+02  | 0.13369907E-01  | 0.04671953E-04  |    |         |         |         | 3 |
| -0.11281401E-07 | 0.04263566E-10  | -0.02124588E+06 | 0.13350887E+02  |                 |    |         |         |         | 4 |
| CH3O            | 121686C         | 1H              | 30              | 1               | G  | 0300.00 | 3000.00 | 1000.00 | 1 |
| 0.03770799E+02  | 0.07871497E-01  | -0.02656384E-04 | 0.03944431E-08  | -0.02112616E-12 |    |         |         |         | 2 |
| 0.12783252E+03  | 0.02929575E+02  | 0.02106204E+02  | 0.07216595E-01  | 0.05338472E-04  |    |         |         |         | 3 |
| -0.07377636E-07 | 0.02075610E-10  | 0.09786011E+04  | 0.13152177E+02  |                 |    |         |         |         | 4 |
| CH3OH           | 121686C         | 1H              | 40              | 1               | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.04029061E+02  | 0.09376593E-01  | -0.03050254E-04 | 0.04358793E-08  | -0.02224723E-12 |    |         |         |         | 2 |
| -0.02615791E+06 | 0.02378195E+02  | 0.02660115E+02  | 0.07341508E-01  | 0.07170050E-04  |    |         |         |         | 3 |
| -0.08793194E-07 | 0.02390570E-10  | -0.02535348E+06 | 0.11232631E+02  |                 |    |         |         |         | 4 |
| CH3SICL3        | 112989C         | 1H              | 3CL             | 3SI             | 1G | 0300.00 | 1500.00 | 1000.00 | 1 |
| 0.11803988E+02  | 0.07642902E-01  | -0.09493348E-06 | -0.01852654E-07 | 0.05302190E-11  |    |         |         |         | 2 |
| -0.06773651E+06 | -0.02794492E+03 | 0.04637712E+02  | 0.03733016E+00  | -0.04798528E-03 |    |         |         |         | 3 |
| 0.03353132E-06  | -0.09484405E-10 | -0.06629348E+06 | 0.06524867E+02  |                 |    |         |         |         | 4 |
| CH4             | 121286C         | 1H              | 4               |                 | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.01683478E+02  | 0.10237236E-01  | -0.03875128E-04 | 0.06785585E-08  | -0.04503423E-12 |    |         |         |         | 2 |
| -0.10080787E+05 | 0.09623395E+02  | 0.07787415E+01  | 0.01747668E+00  | -0.02783409E-03 |    |         |         |         | 3 |
| 0.03049708E-06  | -0.12239307E-10 | -0.09825229E+05 | 0.13722195E+02  |                 |    |         |         |         | 4 |
| CHCL            | 112989C         | 1H              | 1CL             | 1               | G  | 0300.00 | 5000.00 | 1200.00 | 1 |
| 0.03216518E+02  | 0.05976969E-01  | -0.02918238E-04 | 0.05912801E-08  | -0.04297945E-12 |    |         |         |         | 2 |
| 0.03879839E+06  | 0.07793842E+02  | 0.02781262E+02  | 0.07805384E-01  | -0.10637111E-04 |    |         |         |         | 3 |
| 0.10654407E-07  | -0.03916796E-10 | 0.03916144E+06  | 0.10455153E+02  |                 |    |         |         |         | 4 |
| CHCL3           | 112989C         | 1H              | 1CL             | 3               | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.08523544E+02  | 0.04480142E-01  | -0.01837282E-04 | 0.03424891E-08  | -0.02387283E-12 |    |         |         |         | 2 |
| -0.15461167E+05 | -0.15056193E+02 | 0.03437633E+02  | 0.01941496E+00  | -0.16494730E-04 |    |         |         |         | 3 |
| 0.05196545E-07  | -0.06939614E-12 | -0.14161262E+05 | 0.10863299E+02  |                 |    |         |         |         | 4 |
| CHF             | 82489C          | 1H              | 1F              | 1               | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.04242812E+02  | 0.02066316E-01  | -0.06527951E-05 | 0.13887000E-09  | -0.12133360E-13 |    |         |         |         | 2 |
| 0.13559817E+05  | 0.01680196E+02  | 0.03029060E+02  | 0.04850873E-01  | -0.04971678E-04 |    |         |         |         | 3 |
| 0.05277968E-07  | -0.02403154E-10 | 0.14014348E+05  | 0.08324101E+02  |                 |    |         |         |         | 4 |
| CHF3            | 82489C          | 1H              | 1F              | 3               | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.06834333E+02  | 0.06248730E-01  | -0.02575750E-04 | 0.04809112E-08  | -0.03352074E-12 |    |         |         |         | 2 |
| -0.08663771E+06 | -0.10627405E+02 | 0.08725142E+01  | 0.02308431E+00  | -0.02123718E-03 |    |         |         |         | 3 |
| 0.11144284E-07  | -0.02909229E-10 | -0.08496391E+06 | 0.02021498E+03  |                 |    |         |         |         | 4 |
| CL              | 42189CL         | 1               |                 |                 | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.02920236E+02  | -0.03597985E-02 | 0.12942943E-06  | -0.02162776E-09 | 0.13765171E-14  |    |         |         |         | 2 |
| 0.13713381E+05  | 0.03262690E+02  | 0.02381576E+02  | 0.08891079E-02  | 0.04070475E-05  |    |         |         |         | 3 |
| -0.02168943E-07 | 0.11608274E-11  | 0.13839987E+05  | 0.06021817E+02  |                 |    |         |         |         | 4 |
| CL2             | 42189CL         | 2               |                 |                 | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.04274586E+02  | 0.03717336E-02  | -0.01893489E-05 | 0.05337465E-09  | -0.05057602E-13 |    |         |         |         | 2 |
| -0.13311486E+04 | 0.02256946E+02  | 0.03439587E+02  | 0.02870774E-01  | -0.02385870E-04 |    |         |         |         | 3 |
| 0.02892918E-08  | 0.02915057E-11  | -0.11317875E+04 | 0.06471359E+02  |                 |    |         |         |         | 4 |
| CN              | 121286C         | 1N              | 1               |                 | G  | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.03720119E+02  | 0.15183506E-03  | 0.01987381E-05  | -0.03798371E-09 | 0.13282296E-14  |    |         |         |         | 2 |
| 0.05111626E+06  | 0.02888597E+02  | 0.03663204E+02  | -0.11565290E-02 | 0.02163409E-04  |    |         |         |         | 3 |
| 0.01854208E-08  | -0.08214695E-11 | 0.05128118E+06  | 0.03739015E+02  |                 |    |         |         |         | 4 |

|      |                 |                 |                 |                 |                 |         |         |         |   |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| CN+  | 121286C         | 1N              | 1E              | -1              | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.03701463E+02  | 0.07482931E-02  | -0.01790173E-05 | 0.02366368E-09  | -0.14370368E-14 |         |         |         | 2 |
|      | 0.02155966E+07  | 0.04108678E+02  | 0.03118657E+02  | 0.15532581E-02  | -0.09487764E-05 |         |         |         | 3 |
|      | 0.14795005E-08  | -0.09096763E-11 | 0.02158512E+07  | 0.07456254E+02  |                 |         |         |         | 4 |
| CN-  | 121286C         | 1N              | 1E              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02981276E+02  | 0.14647728E-02  | -0.05672737E-05 | 0.10176226E-09  | -0.06870930E-13 |         |         |         | 2 |
|      | 0.06346098E+05  | 0.06171693E+02  | 0.03278995E+02  | 0.14641916E-02  | -0.03925899E-04 |         |         |         | 3 |
|      | 0.05629874E-07  | -0.02473496E-10 | 0.06279509E+05  | 0.04568972E+02  |                 |         |         |         | 4 |
| CN2  | 121686C         | 1N              | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05567064E+02  | 0.02100501E-01  | -0.09010517E-05 | 0.01718571E-08  | -0.12062552E-13 |         |         |         | 2 |
|      | 0.05489968E+06  | -0.05630054E+02 | 0.03039963E+02  | 0.08812105E-01  | -0.07605508E-04 |         |         |         | 3 |
|      | 0.03554357E-07  | -0.08746100E-11 | 0.05563268E+06  | 0.07555298E+02  |                 |         |         |         | 4 |
| CNN  | 121286C         | 1N              | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.04785930E+02  | 0.02559553E-01  | -0.10031326E-05 | 0.01807148E-08  | -0.12273827E-13 |         |         |         | 2 |
|      | 0.06870411E+06  | -0.02953957E+01 | 0.03524436E+02  | 0.07271923E-01  | -0.08272698E-04 |         |         |         | 3 |
|      | 0.05628704E-07  | -0.16415759E-11 | 0.06899647E+06  | 0.05932444E+02  |                 |         |         |         | 4 |
| CO   | 121286C         | 10              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.03025078E+02  | 0.14426885E-02  | -0.05630827E-05 | 0.10185813E-09  | -0.06910951E-13 |         |         |         | 2 |
|      | -0.14268350E+05 | 0.06108217E+02  | 0.03262451E+02  | 0.15119409E-02  | -0.03881755E-04 |         |         |         | 3 |
|      | 0.05581944E-07  | -0.02474951E-10 | -0.14310539E+05 | 0.04848897E+02  |                 |         |         |         | 4 |
| CO2  | 121286C         | 10              | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.04453623E+02  | 0.03140168E-01  | -0.12784105E-05 | 0.02393996E-08  | -0.16690333E-13 |         |         |         | 2 |
|      | -0.04896696E+06 | -0.09553959E+01 | 0.02275724E+02  | 0.09922072E-01  | -0.10409113E-04 |         |         |         | 3 |
|      | 0.06866686E-07  | -0.02117280E-10 | -0.04837314E+06 | 0.10188488E+02  |                 |         |         |         | 4 |
| CO2- | 121286C         | 10              | 2E              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.04610574E+02  | 0.02532962E-01  | -0.10701653E-05 | 0.02026770E-08  | -0.14249581E-13 |         |         |         | 2 |
|      | -0.05479881E+06 | 0.14496295E+01  | 0.02637077E+02  | 0.07803230E-01  | -0.08196187E-04 |         |         |         | 3 |
|      | 0.06537897E-07  | -0.02520220E-10 | -0.05416772E+06 | 0.11889549E+02  |                 |         |         |         | 4 |
| COS  | 121286C         | 10              | 1S              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05191924E+02  | 0.02506123E-01  | -0.10243963E-05 | 0.01943914E-08  | -0.13707999E-13 |         |         |         | 2 |
|      | -0.01846210E+06 | -0.02825755E+02 | 0.02858530E+02  | 0.09515458E-01  | -0.08884915E-04 |         |         |         | 3 |
|      | 0.04220994E-07  | -0.08557340E-11 | -0.01785144E+06 | 0.09081989E+02  |                 |         |         |         | 4 |
| CS   | 121686C         | 1S              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.03737430E+02  | 0.08180451E-02  | -0.03178918E-05 | 0.05356801E-09  | -0.02886194E-13 |         |         |         | 2 |
|      | 0.03247725E+06  | 0.03576556E+02  | 0.02938623E+02  | 0.02724351E-01  | -0.02397706E-04 |         |         |         | 3 |
|      | 0.01689500E-07  | -0.06665050E-11 | 0.03273992E+06  | 0.07848720E+02  |                 |         |         |         | 4 |
| CS2  | 121286C         | 1S              | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05930515E+02  | 0.01813645E-01  | -0.07492172E-05 | 0.14458920E-09  | -0.10326380E-13 |         |         |         | 2 |
|      | 0.12051166E+05  | -0.06093909E+02 | 0.03566139E+02  | 0.08374927E-01  | -0.06835704E-04 |         |         |         | 3 |
|      | 0.02091214E-07  | -0.06737193E-12 | 0.12688482E+05  | 0.06085967E+02  |                 |         |         |         | 4 |
| E    | 120186E         | 1               |                 |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 2 |
|      | -0.07453749E+04 | -0.11734026E+02 | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 3 |
|      | 0.00000000E+00  | 0.00000000E+00  | -0.07453750E+04 | -0.11734026E+02 |                 |         |         |         | 4 |
| F    | 121286F         | 1               |                 |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02687459E+02  | -0.02010358E-02 | 0.08597957E-06  | -0.16449738E-10 | 0.11661605E-14  |         |         |         | 2 |
|      | 0.08722883E+05  | 0.03882212E+02  | 0.02913904E+02  | -0.07336339E-02 | 0.05571015E-05  |         |         |         | 3 |
|      | -0.02666871E-08 | 0.08643255E-12  | 0.08651201E+05  | 0.02677115E+02  |                 |         |         |         | 4 |

|           |                 |                 |                 |                 |                 |         |         |         |
|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|
| F2        | 121286F         | 2               |                 | G               | 0300.00         | 5000.00 | 1000.00 | 1       |
|           | 0.04018308E+02  | 0.06221479E-02  | -0.02420845E-05 | 0.04742076E-09  | -0.03418141E-13 |         |         | 2       |
|           | -0.13007128E+04 | 0.11263273E+01  | 0.02940287E+02  | 0.03491491E-01  | -0.02458207E-04 |         |         | 3       |
|           | 0.01837073E-08  | 0.02850916E-11  | -0.10104296E+04 | 0.06694194E+02  |                 |         |         | 4       |
| F2SINH    | 42489SI         | 1N              | 1F              | 2H              | 1G              | 0300.00 | 3000.00 | 1000.00 |
|           | 0.10048301E+02  | 0.01983144E-01  | -0.02703168E-05 | -0.01767852E-08 | 0.04444367E-12  |         |         | 2       |
|           | -0.07739741E+06 | -0.02303888E+03 | 0.04951547E+02  | 0.13296361E-01  | -0.02098648E-04 |         |         | 3       |
|           | -0.10072757E-07 | 0.05552285E-10  | -0.07597540E+06 | 0.03690891E+02  |                 |         |         | 4       |
| F3SIN     | 22790F          | 3SI             | 1N              | 1               | G               | 0300.00 | 4000.00 | 1000.00 |
|           | 0.11512423E+02  | 0.11150295E-02  | -0.16054655E-06 | -0.05271933E-09 | 0.11608998E-13  |         |         | 2       |
|           | -0.10459191E+06 | -0.02981224E+03 | 0.06028419E+02  | 0.12786807E-01  | -0.01878856E-04 |         |         | 3       |
|           | -0.09695426E-07 | 0.05184847E-10  | -0.10299499E+06 | -0.08217830E+01 |                 |         |         | 4       |
| FNNF      | 42489F          | 2N              | 2               |                 | G               | 0300.00 | 3000.00 | 1000.00 |
|           | 0.07255211E+02  | 0.02274409E-01  | -0.02793346E-05 | -0.02203843E-08 | 0.05359234E-12  |         |         | 2       |
|           | 0.06360352E+05  | -0.10942477E+02 | 0.03127143E+02  | 0.10571342E-01  | -0.09746113E-05 |         |         | 3       |
|           | -0.07208357E-07 | 0.03567978E-10  | 0.07615830E+05  | 0.11074648E+02  |                 |         |         | 4       |
| FNO3      | 121286F         | 1N              | 10              | 3               | G               | 0300.00 | 5000.00 | 1000.00 |
|           | 0.09176275E+02  | 0.04219072E-01  | -0.01835575E-04 | 0.03553717E-08  | -0.02541078E-12 |         |         | 2       |
|           | -0.02118638E+05 | -0.01934397E+03 | 0.02985786E+02  | 0.02094642E+00  | -0.16527329E-04 |         |         | 3       |
|           | 0.04318770E-07  | 0.16607836E-12  | -0.04237215E+04 | 0.12667929E+02  |                 |         |         | 4       |
| FO        | 121286F         | 10              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 |
|           | 0.03913735E+02  | 0.07210714E-02  | -0.02796614E-05 | 0.05337821E-09  | -0.03720183E-13 |         |         | 2       |
|           | 0.11801406E+05  | 0.03346367E+02  | 0.02879578E+02  | 0.03399121E-01  | -0.02572854E-04 |         |         | 3       |
|           | 0.07422381E-08  | -0.04328053E-12 | 0.12096633E+05  | 0.08738887E+02  |                 |         |         | 4       |
| FO2       | 121286F         | 10              | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 |
|           | 0.05678971E+02  | 0.14424551E-02  | -0.06229546E-05 | 0.11996118E-09  | -0.08543416E-13 |         |         | 2       |
|           | -0.03861836E+04 | -0.01941811E+02 | 0.03872542E+02  | 0.06409974E-01  | -0.05517784E-04 |         |         | 3       |
|           | 0.02232770E-07  | -0.03876157E-11 | 0.11570760E+03  | 0.07406949E+02  |                 |         |         | 4       |
| FSIN      | 42489SI         | 1N              | 1F              | 1               | G               | 0300.00 | 3000.00 | 1000.00 |
|           | 0.06269572E+02  | 0.06747867E-02  | -0.12419759E-06 | -0.04970158E-09 | 0.14244521E-13  |         |         | 2       |
|           | 0.02533350E+06  | -0.04201141E+02 | 0.04269969E+02  | 0.05298358E-01  | -0.11038015E-05 |         |         | 3       |
|           | -0.03962805E-07 | 0.02282982E-10  | 0.02587238E+06  | 0.06215038E+02  |                 |         |         | 4       |
| GA        | 62987GA         | 1               |                 |                 | G               | 0300.00 | 1500.00 | 0600.00 |
|           | 0.02679919E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         | 2       |
|           | 0.03368804E+06  | 0.06788109E+02  | 0.02679919E+02  | 0.00000000E+00  | 0.00000000E+00  |         |         | 3       |
|           | 0.00000000E+00  | 0.00000000E+00  | 0.03368803E+06  | 0.06788109E+02  |                 |         |         | 4       |
| GA2H6     | 62987GA         | 2H              | 6               |                 | G               | 0300.00 | 1500.00 | 0600.00 |
|           | 0.06016247E+02  | 0.01788370E+00  | -0.12042288E-06 | -0.06487881E-07 | 0.02075367E-10  |         |         | 2       |
|           | 0.13125479E+05  | -0.05228029E+02 | -0.03914560E+02 | 0.04965434E+00  | 0.07401903E-04  |         |         | 3       |
|           | -0.11241373E-06 | 0.08726339E-09  | 0.14930795E+05  | 0.04274882E+03  |                 |         |         | 4       |
| GAAS      | 62987GA         | 1AS             | 1               |                 | G               | 0300.00 | 1500.00 | 0600.00 |
|           | 0.04471149E+02  | 0.04238449E-02  | -0.02279404E-05 | -0.04441172E-10 | 0.02618952E-12  |         |         | 2       |
|           | 0.04313359E+06  | 0.06212470E+02  | 0.03967473E+02  | 0.02318966E-01  | -0.11454521E-05 |         |         | 3       |
|           | -0.03411430E-07 | 0.03365821E-10  | 0.04321919E+06  | 0.08599628E+02  |                 |         |         | 4       |
| GAAS(3,C) | 62987GA         | 3AS             | 3               |                 | G               | 0300.00 | 1500.00 | 0600.00 |
|           | 0.14852467E+02  | 0.02959435E-01  | -0.07124246E-05 | -0.05316048E-08 | 0.12873211E-12  |         |         | 2       |
|           | 0.11912617E+06  | -0.03514144E+03 | 0.14701892E+02  | 0.03827728E-01  | -0.02945747E-04 |         |         | 3       |
|           | 0.02465370E-07  | -0.15205979E-11 | 0.11914958E+06  | -0.03445955E+03 |                 |         |         | 4       |

|                 |                 |                 |                 |                 |         |         |         |   |
|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| GAAS(3,L)       | 62987GA         | 3AS             | 3               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.13568498E+02  | 0.02802435E-01  | -0.07969918E-05 | -0.06437098E-08 | 0.15602546E-12  |         |         |         | 2 |
| 0.12480055E+06  | -0.13810628E+02 | 0.13412763E+02  | 0.03617689E-01  | -0.02726208E-04 |         |         |         | 3 |
| 0.01877183E-07  | -0.12591780E-11 | 0.12482649E+06  | -0.13091947E+02 |                 |         |         |         | 4 |
| GAAS(5,C)       | 62987GA         | 5AS             | 5               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.02573672E+03  | 0.05523956E-01  | -0.12034680E-05 | -0.10437431E-08 | 0.02528930E-11  |         |         |         | 2 |
| 0.01721381E+07  | -0.08254488E+03 | 0.02546511E+03  | 0.07014337E-01  | -0.04881356E-04 |         |         |         | 3 |
| 0.03825484E-07  | -0.02450420E-10 | 0.01721819E+07  | -0.08130267E+03 |                 |         |         |         | 4 |
| GAAS(5,L)       | 62987GA         | 5AS             | 5               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.03045793E+03  | 0.05403151E-01  | -0.16494765E-05 | -0.09968843E-08 | 0.02413154E-11  |         |         |         | 2 |
| 0.02020691E+07  | -0.07768010E+03 | 0.03015255E+03  | 0.07234394E-01  | -0.06497993E-04 |         |         |         | 3 |
| 0.05559584E-07  | -0.03339653E-10 | 0.02021150E+07  | -0.07630866E+03 |                 |         |         |         | 4 |
| GAET            | 62987GA         | 1C              | 2H 5            | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.05932970E+02  | 0.13424544E-01  | 0.04110518E-05  | -0.04286069E-07 | 0.12387095E-11  |         |         |         | 2 |
| 0.06504863E+05  | 0.03090838E+02  | 0.01846399E+02  | 0.02592050E+00  | 0.05522393E-04  |         |         |         | 3 |
| -0.04977960E-06 | 0.03654361E-09  | 0.07264445E+05  | 0.02294638E+03  |                 |         |         |         | 4 |
| GAET2           | 62987GA         | 1C              | 4H 10           | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.07213832E+02  | 0.03055227E+00  | 0.12494508E-05  | -0.09990274E-07 | 0.02881965E-10  |         |         |         | 2 |
| -0.13921194E+04 | -0.07795098E+00 | -0.02162930E+02 | 0.05892512E+00  | 0.14471449E-04  |         |         |         | 3 |
| -0.11686023E-06 | 0.08526654E-09  | 0.03561840E+04  | 0.04552626E+03  |                 |         |         |         | 4 |
| GAET3           | 62987GA         | 1C              | 6H 15           | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.08436453E+02  | 0.04804950E+00  | 0.02119157E-04  | -0.15816849E-07 | 0.04571178E-10  |         |         |         | 2 |
| -0.13469963E+05 | -0.06196490E+02 | -0.06544288E+02 | 0.09332246E+00  | 0.02364121E-03  |         |         |         | 3 |
| -0.01874104E-05 | 0.13677210E-09  | -0.10676594E+05 | 0.06666796E+03  |                 |         |         |         | 4 |
| GAH             | 62987GA         | 1H              | 1               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.03232142E+02  | 0.13432469E-02  | -0.04325498E-06 | -0.02791841E-08 | 0.04973590E-12  |         |         |         | 2 |
| 0.02656059E+06  | 0.05947896E+02  | 0.03524579E+02  | 0.03386213E-02  | -0.02064013E-05 |         |         |         | 3 |
| 0.03220998E-07  | -0.02936132E-10 | 0.02651074E+06  | 0.04554066E+02  |                 |         |         |         | 4 |
| GAH2            | 62987GA         | 1H              | 2               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.03762384E+02  | 0.03210792E-01  | 0.02180096E-06  | -0.08908394E-08 | 0.02219062E-11  |         |         |         | 2 |
| 0.01936646E+06  | 0.05783398E+02  | 0.03559710E+02  | 0.03676741E-01  | 0.06484499E-05  |         |         |         | 3 |
| -0.03109349E-07 | 0.15854136E-11  | 0.01940976E+06  | 0.06803081E+02  |                 |         |         |         | 4 |
| GAH3            | 62987GA         | 1H              | 3               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.03345475E+02  | 0.06399313E-01  | 0.11229964E-06  | -0.02065899E-07 | 0.05780202E-11  |         |         |         | 2 |
| 0.12281851E+05  | 0.06394841E+02  | 0.01726153E+02  | 0.11247386E-01  | 0.02447526E-04  |         |         |         | 3 |
| -0.02026314E-06 | 0.14470000E-10  | 0.12586196E+05  | 0.14284450E+02  |                 |         |         |         | 4 |
| GAME            | 62987GA         | 1C              | 1H 3            | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.04809857E+02  | 0.06824206E-01  | 0.02258235E-05  | -0.02018341E-07 | 0.05736453E-11  |         |         |         | 2 |
| 0.07558677E+05  | 0.02595904E+02  | 0.03054536E+02  | 0.12186402E-01  | 0.02332213E-04  |         |         |         | 3 |
| -0.02121866E-06 | 0.15442261E-10  | 0.07885868E+05  | 0.11128781E+02  |                 |         |         |         | 4 |
| GAME2           | 62987GA         | 1C              | 2H 6            | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.07068372E+02  | 0.14216021E-01  | 0.05120694E-05  | -0.04421986E-07 | 0.13096413E-11  |         |         |         | 2 |
| 0.05453790E+05  | -0.04173960E+02 | 0.02257655E+02  | 0.02916445E+00  | 0.05669861E-04  |         |         |         | 3 |
| -0.05709755E-06 | 0.04268905E-09  | 0.06341297E+05  | 0.01915435E+03  |                 |         |         |         | 4 |
| GAME3           | 62987GA         | 1C              | 3H 9            | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.08410636E+02  | 0.02262803E+00  | 0.10430190E-05  | -0.07049610E-07 | 0.02015307E-10  |         |         |         | 2 |
| -0.09087271E+05 | -0.10722496E+02 | 0.02120238E+02  | 0.04161029E+00  | 0.09959505E-04  |         |         |         | 3 |
| -0.07846792E-06 | 0.05693396E-09  | -0.07911968E+05 | 0.01988516E+03  |                 |         |         |         | 4 |

|          |                 |                 |                 |                 |                 |                |                |         |
|----------|-----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|---------|
| H        | 120186H         | 1               |                 | G               | 0300.00         | 5000.00        | 1000.00        | 1       |
|          | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00 | 2       |
|          | 0.02547162E+06  | -0.04601176E+01 | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00 | 3       |
|          | 0.00000000E+00  | 0.00000000E+00  | 0.02547162E+06  | -0.04601176E+01 |                 |                |                | 4       |
| H+       | 120186H         | 1E              | -1              | G               | 0300.00         | 5000.00        | 1000.00        | 1       |
|          | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00 | 2       |
|          | 0.01840334E+07  | -0.11538620E+01 | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00 | 3       |
|          | 0.00000000E+00  | 0.00000000E+00  | 0.01840334E+07  | -0.11538621E+01 |                 |                |                | 4       |
| H-       | 120186H         | 1E              | 1               | G               | 0300.00         | 5000.00        | 1000.00        | 1       |
|          | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00 | 2       |
|          | 0.15961045E+05  | -0.11524488E+01 | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00 | 3       |
|          | 0.00000000E+00  | 0.00000000E+00  | 0.15961045E+05  | -0.11524486E+01 |                 |                |                | 4       |
| H2       | 121286H         | 2               |                 | G               | 0300.00         | 5000.00        | 1000.00        | 1       |
|          | 0.02991423E+02  | 0.07000644E-02  | -0.05633828E-06 | -0.09231578E-10 | 0.15827519E-14  |                |                | 2       |
|          | -0.08350340E+04 | -0.13551101E+01 | 0.03298124E+02  | 0.08249441E-02  | -0.08143015E-05 |                |                | 3       |
|          | -0.09475434E-09 | 0.04134872E-11  | -0.10125209E+04 | -0.03294094E+02 |                 |                |                | 4       |
| H2ALME   | 62987AL         | 1C              | 1H              | 5               | G               | 0300.00        | 1500.00        | 0600.00 |
|          | 0.04898410E+02  | 0.13582233E-01  | 0.02611458E-05  | -0.04575170E-07 | 0.13848023E-11  |                |                | 2       |
|          | 0.08743072E+04  | -0.11131169E+01 | -0.06283259E+01 | 0.03089530E+00  | 0.05774090E-04  |                |                | 3       |
|          | -0.06488033E-06 | 0.04907111E-09  | 0.01889333E+05  | 0.02565779E+03  |                 |                |                | 4       |
| H2ASME   | 62987AS         | 1C              | 1H              | 5               | G               | 0300.00        | 1500.00        | 0600.00 |
|          | 0.05686213E+02  | 0.02154421E+00  | 0.08185247E-05  | -0.07069951E-07 | 0.02101522E-10  |                |                | 2       |
|          | 0.09331084E+05  | -0.06513957E+02 | -0.02113506E+02 | 0.04564229E+00  | 0.09983227E-04  |                |                | 3       |
|          | -0.09399697E-06 | 0.07014021E-09  | 0.10771701E+05  | 0.03132610E+03  |                 |                |                | 4       |
| H2C40    | 120189H         | 2C              | 40              | 1               | G               | 0300.00        | 4000.00        | 1000.00 |
|          | 0.10268878E+02  | 0.04896164E-01  | -0.04885080E-05 | -0.02708566E-08 | 0.05107013E-12  |                |                | 2       |
|          | 0.02346902E+06  | -0.02815985E+03 | 0.04810971E+02  | 0.13139988E-01  | 0.09865073E-05  |                |                | 3       |
|          | -0.06120720E-07 | 0.16400028E-11  | 0.02545803E+06  | 0.02113424E+02  |                 |                |                | 4       |
| H2CCCCH  | 82489C          | 4H              | 3               | G               | 0300.00         | 4000.00        | 1000.00        | 1       |
|          | 0.11314095E+02  | 0.05014414E-01  | -0.05350444E-05 | -0.02825309E-08 | 0.05403279E-12  |                |                | 2       |
|          | 0.05181211E+06  | -0.03062434E+03 | 0.06545799E+02  | 0.12424768E-01  | 0.05603226E-05  |                |                | 3       |
|          | -0.05631141E-07 | 0.16652183E-11  | 0.05352502E+06  | -0.04264082E+02 |                 |                |                | 4       |
| H2CCCCH2 | 82489C          | 4H              | 4               | G               | 0300.00         | 4000.00        | 1000.00        | 1       |
|          | 0.10620828E+02  | 0.07199370E-01  | -0.06806234E-05 | -0.04021185E-08 | 0.07378498E-12  |                |                | 2       |
|          | 0.03358797E+06  | -0.03193583E+03 | 0.03849007E+02  | 0.01713169E+00  | 0.16442703E-05  |                |                | 3       |
|          | -0.07761590E-07 | 0.01947859E-10  | 0.03608372E+06  | 0.05732120E+02  |                 |                |                | 4       |
| H2CCCH   | 82489C          | 3H              | 3               | G               | 0300.00         | 4000.00        | 1000.00        | 1       |
|          | 0.08831047E+02  | 0.04357194E-01  | -0.04109066E-05 | -0.02368723E-08 | 0.04376520E-12  |                |                | 2       |
|          | 0.03847419E+06  | -0.02177919E+03 | 0.04754199E+02  | 0.11080277E-01  | 0.02793323E-05  |                |                | 3       |
|          | -0.05479212E-07 | 0.01949629E-10  | 0.03988883E+06  | 0.05854549E+01  |                 |                |                | 4       |
| H2CN     | 41687H          | 2C              | 1N              | 1               | G               | 0300.00        | 4000.00        | 1000.00 |
|          | 0.05209703E+02  | 0.02969291E-01  | -0.02855589E-05 | -0.16355504E-09 | 0.03043259E-12  |                |                | 2       |
|          | 0.02767711E+06  | -0.04444478E+02 | 0.02851661E+02  | 0.05695233E-01  | 0.10711403E-05  |                |                | 3       |
|          | -0.16226120E-08 | -0.02351108E-11 | 0.02863782E+06  | 0.08992751E+02  |                 |                |                | 4       |
| H2CNH    | 41687C          | 1H              | 3N              | 1               | G               | 0300.00        | 4000.00        | 1000.00 |
|          | 0.05221589E+02  | 0.04748525E-01  | -0.04179158E-05 | -0.02606612E-08 | 0.04703140E-12  |                |                | 2       |
|          | 0.08657219E+05  | -0.04500776E+02 | 0.02365878E+02  | 0.06780570E-01  | 0.02422999E-04  |                |                | 3       |
|          | -0.06157824E-08 | -0.16150971E-11 | 0.09971141E+05  | 0.12307176E+02  |                 |                |                | 4       |

|            |                 |                 |                 |                 |                 |         |         |         |   |
|------------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| H2CNN02    | 41687H          | 2C              | 1N              | 20              | 2G              | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.11407942E+02  | 0.04564542E-01  | -0.04600304E-05 | -0.02513538E-08 | 0.04782211E-12  |         |         |         | 2 |
|            | 0.12421422E+05  | -0.03165237E+03 | 0.03534316E+02  | 0.01811271E+00  | 0.02394017E-05  |         |         |         | 3 |
|            | -0.10800240E-07 | 0.04222725E-10  | 0.15090057E+05  | 0.11311378E+02  |                 |         |         |         | 4 |
| H2GAET     | 62987GA         | 1C              | 2H              | 7               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|            | 0.07187273E+02  | 0.01867211E+00  | 0.06156157E-05  | -0.06027763E-07 | 0.01797524E-10  |         |         |         | 2 |
|            | -0.04232757E+05 | -0.04686699E+02 | 0.04124020E+01  | 0.03972971E+00  | 0.07979140E-04  |         |         |         | 3 |
|            | -0.08059233E-06 | 0.06040387E-09  | -0.02983932E+05 | 0.02816147E+03  |                 |         |         |         | 4 |
| H2GAME     | 62987GA         | 1C              | 1H              | 5               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|            | 0.05831604E+02  | 0.12228715E-01  | 0.03033669E-05  | -0.03956941E-07 | 0.12254516E-11  |         |         |         | 2 |
|            | 0.05189255E+05  | -0.04446614E+02 | 0.05251130E+01  | 0.02904695E+00  | 0.04844148E-04  |         |         |         | 3 |
|            | -0.06097646E-06 | 0.04672763E-09  | 0.06158712E+05  | 0.02122148E+03  |                 |         |         |         | 4 |
| H2NF       | 42489H          | 2N              | 1F              | 1               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|            | 0.04143658E+02  | 0.03805135E-01  | -0.02771153E-05 | -0.03589717E-08 | 0.07589549E-12  |         |         |         | 2 |
|            | -0.04891486E+05 | 0.02309362E+02  | 0.02597862E+02  | 0.05882104E-01  | 0.04938351E-05  |         |         |         | 3 |
|            | -0.01948600E-07 | 0.03634002E-11  | -0.04301253E+05 | 0.10982895E+02  |                 |         |         |         | 4 |
| H2O        | 20387H          | 20              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.02672145E+02  | 0.03056293E-01  | -0.08730260E-05 | 0.12009964E-09  | -0.06391618E-13 |         |         |         | 2 |
|            | -0.02989921E+06 | 0.06862817E+02  | 0.03386842E+02  | 0.03474982E-01  | -0.06354696E-04 |         |         |         | 3 |
|            | 0.06968581E-07  | -0.02506588E-10 | -0.03020811E+06 | 0.02590232E+02  |                 |         |         |         | 4 |
| H2O(L)     | 120186H         | 20              | 1               |                 | L               | 0273.15 | 1000.00 | 1000.00 | 1 |
|            | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 2 |
|            | 0.00000000E+00  | 0.00000000E+00  | 0.12712782E+02  | -0.01766279E+00 | -0.02255666E-03 |         |         |         | 3 |
|            | 0.02082090E-05  | -0.02407861E-08 | -0.03748320E+06 | -0.05911534E+03 |                 |         |         |         | 4 |
| H2O(S)     | 120186H         | 20              | 1               |                 | S               | 0200.00 | 0273.15 | 1000.00 | 1 |
|            | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 2 |
|            | 0.00000000E+00  | 0.00000000E+00  | -0.03926933E+00 | 0.01692042E+00  | 0.00000000E+00  |         |         |         | 3 |
|            | 0.00000000E+00  | 0.00000000E+00  | -0.03594958E+06 | 0.05693378E+01  |                 |         |         |         | 4 |
| H2O2       | 120186H         | 20              | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.04573167E+02  | 0.04336136E-01  | -0.14746888E-05 | 0.02348903E-08  | -0.14316536E-13 |         |         |         | 2 |
|            | -0.01800696E+06 | 0.05011369E+01  | 0.03388753E+02  | 0.06569226E-01  | -0.14850125E-06 |         |         |         | 3 |
|            | -0.04625805E-07 | 0.02471514E-10  | -0.01766314E+06 | 0.06785363E+02  |                 |         |         |         | 4 |
| H2S        | 121286H         | 2S              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.02883147E+02  | 0.03827835E-01  | -0.14233978E-05 | 0.02497998E-08  | -0.16602733E-13 |         |         |         | 2 |
|            | -0.03480742E+05 | 0.07258161E+02  | 0.03071029E+02  | 0.05578261E-01  | -0.10309669E-04 |         |         |         | 3 |
|            | 0.12019529E-07  | -0.04838369E-10 | -0.03559826E+05 | 0.05935226E+02  |                 |         |         |         | 4 |
| H2SI(NH2)2 | 22790SI         | 1H              | 6N              | 2               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.13021791E+02  | 0.06465444E-01  | -0.05816746E-05 | -0.03484493E-08 | 0.06340675E-12  |         |         |         | 2 |
|            | -0.02357070E+06 | -0.04132569E+03 | 0.05615307E+02  | 0.02079854E+00  | -0.09999531E-05 |         |         |         | 3 |
|            | -0.12885246E-07 | 0.06091865E-10  | -0.02126283E+06 | -0.16156578E+01 |                 |         |         |         | 4 |
| H2SIN      | 22790H          | 2SI             | 1N              | 1               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.06826533E+02  | 0.02125460E-01  | -0.02343131E-05 | -0.11663394E-09 | 0.02277273E-12  |         |         |         | 2 |
|            | 0.07253672E+06  | -0.10521624E+02 | 0.03549344E+02  | 0.07311004E-01  | 0.03249025E-05  |         |         |         | 3 |
|            | -0.03682945E-07 | 0.11215113E-11  | 0.07370656E+06  | 0.07565328E+02  |                 |         |         |         | 4 |
| H2SINH     | 42489SI         | 1N              | 1H              | 3               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|            | 0.06588295E+02  | 0.04903194E-01  | -0.04944719E-05 | -0.05014630E-08 | 0.11394698E-12  |         |         |         | 2 |
|            | 0.01809794E+06  | -0.09522970E+02 | 0.02822195E+02  | 0.12455182E-01  | -0.08350819E-05 |         |         |         | 3 |
|            | -0.07411813E-07 | 0.03579019E-10  | 0.01923616E+06  | 0.10547831E+02  |                 |         |         |         | 4 |



|                                                                             |          |     |    |    |     |         |         |         |   |
|-----------------------------------------------------------------------------|----------|-----|----|----|-----|---------|---------|---------|---|
| H2SINH2                                                                     | 42489SI  | 1N  | 1H | 4  | G   | 0300.00 | 3000.00 | 1000.00 | 1 |
| 0.07392047E+02 0.05476841E-01-0.04453276E-05-0.05236661E-08 0.11383899E-12  |          |     |    |    |     |         |         |         | 2 |
| 0.11368581E+05-0.11380495E+02 0.04053222E+02 0.11822311E-01-0.04348128E-05  |          |     |    |    |     |         |         |         | 3 |
| -0.06225818E-07 0.02798829E-10 0.12419705E+05 0.06562032E+02                |          |     |    |    |     |         |         |         | 4 |
| H2SINH3                                                                     | 121386SI | 1H  | 5N | 1  | G   | 0300.00 | 4000.00 | 1000.00 | 1 |
| 0.08711392E+02 0.05909106E-01-0.05436615E-05-0.03248350E-08 0.05960257E-12  |          |     |    |    |     |         |         |         | 2 |
| 0.08441694E+05-0.01933470E+03 0.04269729E+02 0.11252245E-01 0.01951721E-04  |          |     |    |    |     |         |         |         | 3 |
| -0.03578372E-07-0.08372202E-12 0.10222041E+05 0.05876735E+02                |          |     |    |    |     |         |         |         | 4 |
| H2SISIH2                                                                    | 42489SI  | 2H  | 4  |    | G   | 0300.00 | 3000.00 | 1000.00 | 1 |
| 0.08986817E+02 0.05405047E-01-0.05214021E-05-0.05313742E-08 0.11887266E-12  |          |     |    |    |     |         |         |         | 2 |
| 0.02832747E+06-0.02004478E+03 0.05133186E+02 0.12528548E-01-0.04620421E-05  |          |     |    |    |     |         |         |         | 3 |
| -0.06606075E-07 0.02864344E-10 0.02956915E+06 0.07605133E+01                |          |     |    |    |     |         |         |         | 4 |
| H3ASGAET3                                                                   | 62987AS  | 1GA | 1C | 6H | 18G | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.08508501E+02 0.05632369E+00 0.02524140E-04-0.01861451E-06 0.05372402E-10  |          |     |    |    |     |         |         |         | 2 |
| -0.10855169E+05-0.03399857E+02-0.08974745E+02 0.10905161E+00 0.02811457E-03 |          |     |    |    |     |         |         |         | 3 |
| -0.02195513E-05 0.15997339E-09-0.07592761E+05 0.08165459E+03                |          |     |    |    |     |         |         |         | 4 |
| H3ASGAME3                                                                   | 62987AS  | 1GA | 1C | 3H | 12G | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.11254990E+02 0.03159752E+00 0.11779036E-05-0.10133524E-07 0.02947355E-10  |          |     |    |    |     |         |         |         | 2 |
| -0.07280344E+05-0.02238729E+03 0.12671606E+01 0.06214586E+00 0.13856307E-04 |          |     |    |    |     |         |         |         | 3 |
| -0.12200444E-06 0.08982019E-09-0.05425619E+05 0.02613306E+03                |          |     |    |    |     |         |         |         | 4 |
| H3SIN                                                                       | 22790H   | 3SI | 1N | 1  | G   | 0300.00 | 4000.00 | 1000.00 | 1 |
| 0.07964213E+02 0.03355633E-01-0.03579695E-05-0.01889818E-08 0.03650912E-12  |          |     |    |    |     |         |         |         | 2 |
| 0.11486972E+06-0.01924110E+03 0.02790628E+02 0.11345662E-01 0.08321879E-05  |          |     |    |    |     |         |         |         | 3 |
| -0.05845045E-07 0.01685969E-10 0.11673571E+06 0.09384630E+02                |          |     |    |    |     |         |         |         | 4 |
| H3SINH                                                                      | 42489SI  | 1N  | 1H | 4  | G   | 0300.00 | 3000.00 | 1000.00 | 1 |
| 0.07697340E+02 0.05657943E-01-0.05209306E-05-0.05617966E-08 0.12635020E-12  |          |     |    |    |     |         |         |         | 2 |
| 0.02282005E+06-0.13303793E+02 0.02778390E+02 0.15107111E-01-0.06734260E-05  |          |     |    |    |     |         |         |         | 3 |
| -0.08928515E-07 0.04115347E-10 0.02435913E+06 0.13093859E+02                |          |     |    |    |     |         |         |         | 4 |
| H3SISIH                                                                     | 90589SI  | 2H  | 4  |    | G   | 0300.00 | 2000.00 | 1000.00 | 1 |
| 0.07778291E+02 0.07255418E-01-0.08123265E-05-0.11682818E-08 0.03425139E-11  |          |     |    |    |     |         |         |         | 2 |
| 0.03742600E+06-0.13484629E+02 0.02774192E+02 0.02555302E+00-0.02883836E-03  |          |     |    |    |     |         |         |         | 3 |
| 0.02000737E-06-0.06100616E-10 0.03861801E+06 0.11350098E+02                 |          |     |    |    |     |         |         |         | 4 |
| H3SISIH3                                                                    | 42489SI  | 2H  | 6  |    | G   | 0300.00 | 3000.00 | 1000.00 | 1 |
| 0.10682729E+02 0.08221416E-01-0.08096035E-05-0.08337975E-08 0.01908205E-11  |          |     |    |    |     |         |         |         | 2 |
| 0.05316920E+05-0.03082188E+03 0.03898289E+02 0.01977415E+00 0.01791014E-05  |          |     |    |    |     |         |         |         | 3 |
| -0.10331682E-07 0.03931698E-10 0.07621719E+05 0.06227022E+02                |          |     |    |    |     |         |         |         | 4 |
| HALME                                                                       | 62987AL  | 1C  | 1H | 4  | G   | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.04812273E+02 0.10296448E-01 0.02582807E-05-0.03323596E-07 0.09884584E-11  |          |     |    |    |     |         |         |         | 2 |
| 0.11766730E+05 0.09557062E+01 0.11187894E+01 0.02180038E+00 0.04120785E-04  |          |     |    |    |     |         |         |         | 3 |
| -0.04366690E-06 0.03273825E-09 0.12447363E+05 0.01886107E+03                |          |     |    |    |     |         |         |         | 4 |
| HALME2                                                                      | 62987AL  | 1C  | 2H | 7  | G   | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.05705171E+02 0.01924317E+00 0.06377855E-05-0.06346800E-07 0.01896799E-10  |          |     |    |    |     |         |         |         | 2 |
| -0.06049864E+05-0.06331378E+01-0.14942614E+01 0.04158567E+00 0.08686772E-04 |          |     |    |    |     |         |         |         | 3 |
| -0.08604142E-06 0.06447652E-09-0.04722516E+05 0.03427724E+03                |          |     |    |    |     |         |         |         | 4 |
| HASALME                                                                     | 62987AS  | 1AL | 1C | 1H | 4G  | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.06956538E+02 0.10612781E-01 0.02440153E-05-0.03297737E-07 0.10200039E-11  |          |     |    |    |     |         |         |         | 2 |
| 0.02582505E+06-0.08625792E+01 0.02544858E+02 0.02465794E+00 0.03677807E-04  |          |     |    |    |     |         |         |         | 3 |
| -0.05008893E-06 0.03848383E-09 0.02663010E+06 0.02046858E+03                |          |     |    |    |     |         |         |         | 4 |

|         |                 |                 |                 |                 |                 |         |         |         |   |
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| HASGAET | 62987AS         | 1GA             | 1C              | 2H              | 6G              | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.06336445E+02  | 0.02340603E+00  | 0.09066638E-05  | -0.07519059E-07 | 0.01828115E-10  |         |         |         | 2 |
|         | 0.03184605E+06  | 0.05812180E+02  | 0.05642723E+02  | 0.02296738E+00  | 0.10948674E-04  |         |         |         | 3 |
|         | -0.02449038E-06 | 0.09602700E-10  | 0.03204717E+06  | 0.09675533E+02  |                 |         |         |         | 4 |
| HASGAME | 62987AS         | 1GA             | 1C              | 1H              | 4G              | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.07507970E+02  | 0.09277900E-01  | 0.01891931E-05  | -0.02769886E-07 | 0.07996069E-11  |         |         |         | 2 |
|         | 0.03253907E+06  | -0.14226081E+01 | 0.04859126E+02  | 0.01750423E+00  | 0.02831995E-04  |         |         |         | 3 |
|         | -0.03107936E-06 | 0.02299468E-09  | 0.03302941E+06  | 0.11429521E+02  |                 |         |         |         | 4 |
| HASME   | 62987AS         | 1C              | 1H              | 4               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.05753261E+02  | 0.01841813E+00  | 0.07493312E-05  | -0.05919916E-07 | 0.01726246E-10  |         |         |         | 2 |
|         | 0.01880057E+06  | -0.05360325E+02 | -0.15750948E+00 | 0.03649094E+00  | 0.08332939E-04  |         |         |         | 3 |
|         | -0.07234666E-06 | 0.05330928E-09  | 0.01989791E+06  | 0.02335316E+03  |                 |         |         |         | 4 |
| HASME2  | 62987AS         | 1C              | 2H              | 7               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.05850436E+02  | 0.01841765E+00  | 0.08066844E-05  | -0.05868715E-07 | 0.01726428E-10  |         |         |         | 2 |
|         | 0.06450535E+05  | 0.03909152E+01  | -0.02908405E+01 | 0.03729576E+00  | 0.08335854E-04  |         |         |         | 3 |
|         | -0.07455611E-06 | 0.05527881E-09  | 0.07587765E+05  | 0.03020451E+03  |                 |         |         |         | 4 |
| HCCCHCH | 82489C          | 4H              | 3               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|         | 0.10752738E+02  | 0.05381153E-01  | -0.05549637E-05 | -0.03052266E-08 | 0.05761740E-12  |         |         |         | 2 |
|         | 0.06121419E+06  | -0.02973025E+03 | 0.04153881E+02  | 0.01726287E+00  | -0.02389374E-05 |         |         |         | 3 |
|         | -0.10187000E-07 | 0.04340504E-10  | 0.06338070E+06  | 0.06036506E+02  |                 |         |         |         | 4 |
| HCCO    | 32387H          | 1C              | 20              | 1               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|         | 0.06758073E+02  | 0.02000400E-01  | -0.02027607E-05 | -0.10411318E-09 | 0.01965164E-12  |         |         |         | 2 |
|         | 0.01901513E+06  | -0.09071262E+02 | 0.05047965E+02  | 0.04453478E-01  | 0.02268282E-05  |         |         |         | 3 |
|         | -0.14820945E-08 | 0.02250741E-11  | 0.01965891E+06  | 0.04818439E+01  |                 |         |         |         | 4 |
| HCCOH   | 32387H          | 2C              | 20              | 1               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|         | 0.07328324E+02  | 0.03336416E-01  | -0.03024705E-05 | -0.01781106E-08 | 0.03245168E-12  |         |         |         | 2 |
|         | 0.07598258E+05  | -0.14012140E+02 | 0.03899465E+02  | 0.09701075E-01  | -0.03119309E-05 |         |         |         | 3 |
|         | -0.05537732E-07 | 0.02465732E-10  | 0.08701190E+05  | 0.04491874E+02  |                 |         |         |         | 4 |
| HCL     | 42189CL         | 1H              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|         | 0.02755335E+02  | 0.14735811E-02  | -0.04971254E-05 | 0.08108658E-09  | -0.05072063E-13 |         |         |         | 2 |
|         | -0.11918058E+05 | 0.06515116E+02  | 0.03338534E+02  | 0.12682066E-02  | -0.03666916E-04 |         |         |         | 3 |
|         | 0.04703992E-07  | -0.01836011E-10 | -0.12131511E+05 | 0.03193555E+02  |                 |         |         |         | 4 |
| HCN     | 121286H         | 1C              | 1N              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|         | 0.03650077E+02  | 0.03460998E-01  | -0.12742788E-05 | 0.02217655E-08  | -0.14771774E-13 |         |         |         | 2 |
|         | 0.14983916E+05  | 0.02393220E+02  | 0.02490462E+02  | 0.08611280E-01  | -0.10310342E-04 |         |         |         | 3 |
|         | 0.07481498E-07  | -0.02229109E-10 | 0.15208344E+05  | 0.07904981E+02  |                 |         |         |         | 4 |
| HCNH    | 41687C          | 1H              | 2N              | 1               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|         | 0.04923292E+02  | 0.03332897E-01  | -0.03370896E-05 | -0.01901619E-08 | 0.03531825E-12  |         |         |         | 2 |
|         | 0.03132669E+06  | -0.16325088E+01 | 0.02759456E+02  | 0.06103386E-01  | 0.07713149E-05  |         |         |         | 3 |
|         | -0.02063093E-07 | 0.01931919E-11  | 0.03217247E+06  | 0.10574895E+02  |                 |         |         |         | 4 |
| HCNO    | 120186H         | 1C              | 1N              | 10              | 1G              | 0250.00 | 4000.00 | 1000.00 | 1 |
|         | 0.06692412E+02  | 0.02368360E-01  | -0.02371510E-05 | -0.12755033E-09 | 0.02407137E-12  |         |         |         | 2 |
|         | 0.01694736E+06  | -0.12454345E+02 | 0.03184858E+02  | 0.09752316E-01  | -0.12802028E-05 |         |         |         | 3 |
|         | -0.06163104E-07 | 0.03226275E-10  | 0.01797907E+06  | 0.06123843E+02  |                 |         |         |         | 4 |
| HCO     | 121286H         | 1C              | 10              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|         | 0.03557271E+02  | 0.03345572E-01  | -0.13350060E-05 | 0.02470572E-08  | -0.01713850E-12 |         |         |         | 2 |
|         | 0.03916324E+05  | 0.05552299E+02  | 0.02898329E+02  | 0.06199146E-01  | -0.09623084E-04 |         |         |         | 3 |
|         | 0.10898249E-07  | -0.04574885E-10 | 0.04159922E+05  | 0.08983614E+02  |                 |         |         |         | 4 |



|         |                 |                 |                 |                 |                 |         |         |         |   |
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| HCO+    | 121286H         | 1C              | 10              | 1E              | -1G             | 0300.00 | 5000.00 | 1000.00 | 1 |
|         | 0.03692074E+02  | 0.03454732E-01  | -0.13165244E-05 | 0.02323551E-08  | -0.15541321E-13 |         |         |         | 2 |
|         | 0.09890941E+06  | 0.02330722E+02  | 0.02496483E+02  | 0.08690658E-01  | -0.10604453E-04 |         |         |         | 3 |
|         | 0.07882791E-07  | -0.02418385E-10 | 0.09915097E+06  | 0.08048177E+02  |                 |         |         |         | 4 |
| HE      | 120186HE        | 1               |                 |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|         | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 2 |
|         | -0.07453750E+04 | 0.09153489E+01  | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 3 |
|         | 0.00000000E+00  | 0.00000000E+00  | -0.07453750E+04 | 0.09153488E+01  |                 |         |         |         | 4 |
| HE+     | 120186HE        | 1E              | -1              |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|         | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 2 |
|         | 0.02853426E+07  | 0.16084045E+01  | 0.02500000E+02  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 3 |
|         | 0.00000000E+00  | 0.00000000E+00  | 0.02853426E+07  | 0.16084046E+01  |                 |         |         |         | 4 |
| HF      | 121286H         | 1F              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|         | 0.02956767E+02  | 0.07721015E-02  | -0.09899834E-06 | -0.04993520E-10 | 0.14293306E-14  |         |         |         | 2 |
|         | -0.03361061E+06 | 0.04011673E+02  | 0.03431841E+02  | 0.04404165E-02  | -0.08828452E-05 |         |         |         | 3 |
|         | 0.06574516E-08  | -0.02055909E-12 | -0.03381977E+06 | 0.12382699E+01  |                 |         |         |         | 4 |
| HGAET   | 62987GA         | 1C              | 2H              | 6               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.06580151E+02  | 0.16101323E-01  | 0.05009545E-05  | -0.05185148E-07 | 0.15240853E-11  |         |         |         | 2 |
|         | 0.08765131E+05  | -0.04046067E+01 | 0.11632838E+01  | 0.03282212E+00  | 0.06765717E-04  |         |         |         | 3 |
|         | -0.06509541E-06 | 0.04835806E-09  | 0.09767174E+05  | 0.02588269E+03  |                 |         |         |         | 4 |
| HGAET2  | 62987GA         | 1C              | 4H              | 11              | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.06511306E+02  | 0.02819753E+00  | 0.14187506E-05  | -0.09000947E-07 | 0.02572894E-10  |         |         |         | 2 |
|         | -0.04482180E+05 | 0.04709021E+02  | -0.14865759E+01 | 0.05217640E+00  | 0.13563420E-04  |         |         |         | 3 |
|         | -0.10119820E-06 | 0.07319853E-09  | -0.02985242E+05 | 0.04364749E+03  |                 |         |         |         | 4 |
| HGAME   | 62987GA         | 1C              | 1H              | 4               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.05318279E+02  | 0.09490931E-01  | 0.02277164E-05  | -0.03005070E-07 | 0.09037830E-11  |         |         |         | 2 |
|         | 0.12535338E+05  | -0.10657105E+00 | 0.01784749E+02  | 0.02058861E+00  | 0.03548509E-04  |         |         |         | 3 |
|         | -0.04111927E-06 | 0.03108978E-09  | 0.13184225E+05  | 0.01700701E+03  |                 |         |         |         | 4 |
| HGAME2  | 62987GA         | 1C              | 2H              | 7               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.06759397E+02  | 0.14261030E-01  | -0.11740239E-06 | -0.05001401E-07 | 0.15027851E-11  |         |         |         | 2 |
|         | -0.14732646E+04 | -0.02967135E+02 | 0.09039155E+01  | 0.03264779E+00  | 0.05389243E-04  |         |         |         | 3 |
|         | -0.06814504E-06 | 0.05150323E-09  | -0.03978242E+04 | 0.02539304E+03  |                 |         |         |         | 4 |
| HMEGAET | 62987GA         | 1C              | 3H              | 9               | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
|         | 0.07025463E+02  | 0.02564787E+00  | 0.09619100E-05  | -0.08403699E-07 | 0.02488960E-10  |         |         |         | 2 |
|         | -0.13613768E+04 | -0.03319484E+02 | -0.02079142E+02 | 0.05373076E+00  | 0.11810364E-04  |         |         |         | 3 |
|         | -0.10998548E-06 | 0.08189554E-09  | 0.03216961E+04  | 0.04086070E+03  |                 |         |         |         | 4 |
| HN3     | 82687H          | 1N              | 3               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|         | 0.06023015E+02  | 0.02454362E-01  | -0.02404279E-05 | -0.13229726E-09 | 0.02474146E-12  |         |         |         | 2 |
|         | 0.03394051E+06  | -0.07015537E+02 | 0.03621003E+02  | 0.06030785E-01  | 0.04054460E-05  |         |         |         | 3 |
|         | -0.02545270E-07 | 0.06174280E-11  | 0.03482373E+06  | 0.06333769E+02  |                 |         |         |         | 4 |
| HNCO    | 31287H          | 1N              | 1C              | 10              | 1G              | 0300.00 | 4000.00 | 1000.00 | 1 |
|         | 0.06211867E+02  | 0.02297137E-01  | -0.02216128E-05 | -0.12220438E-09 | 0.02272406E-12  |         |         |         | 2 |
|         | -0.14770725E+05 | -0.08016633E+02 | 0.03694059E+02  | 0.06657236E-01  | -0.05054468E-06 |         |         |         | 3 |
|         | -0.03473411E-07 | 0.13605694E-11  | -0.13919758E+05 | 0.05712742E+02  |                 |         |         |         | 4 |
| HNF     | 42489H          | 1N              | 1F              | 1               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|         | 0.04133219E+02  | 0.01912056E-01  | -0.16253301E-06 | -0.01726461E-08 | 0.03743691E-12  |         |         |         | 2 |
|         | 0.14670521E+05  | 0.03292122E+02  | 0.03249760E+02  | 0.03261817E-01  | 0.04355642E-06  |         |         |         | 3 |
|         | -0.11002765E-08 | 0.02926757E-11  | 0.14991264E+05  | 0.08187434E+02  |                 |         |         |         | 4 |

|           |                 |                 |                 |                 |                 |         |         |         |   |
|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| HNF2      | 42489H          | 1N              | 1F              | 2               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.05704866E+02  | 0.03049897E-01  | -0.02826802E-05 | -0.02923184E-08 | 0.06551055E-12  |         |         |         | 2 |
|           | -0.09107488E+05 | -0.03941331E+02 | 0.02572812E+02  | 0.08762144E-01  | -0.02326921E-05 |         |         |         | 3 |
|           | -0.05000826E-07 | 0.02143837E-10  | -0.08086760E+05 | 0.13006810E+02  |                 |         |         |         | 4 |
| HNO       | 121286H         | 1N              | 10              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.03615144E+02  | 0.03212485E-01  | -0.12603370E-05 | 0.02267297E-08  | -0.15362358E-13 |         |         |         | 2 |
|           | 0.10661911E+05  | 0.04810263E+02  | 0.02784402E+02  | 0.06609646E-01  | -0.09300223E-04 |         |         |         | 3 |
|           | 0.09437980E-07  | -0.03753146E-10 | 0.10918779E+05  | 0.09035629E+02  |                 |         |         |         | 4 |
| HNO3      | 121286H         | 1N              | 10              | 3               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.07003844E+02  | 0.05811493E-01  | -0.02333788E-04 | 0.04288814E-08  | -0.02959385E-12 |         |         |         | 2 |
|           | -0.01889952E+06 | -0.10478628E+02 | 0.13531850E+01  | 0.02220024E+00  | -0.01978811E-03 |         |         |         | 3 |
|           | 0.08773908E-07  | -0.16583844E-11 | -0.01738562E+06 | 0.01851868E+03  |                 |         |         |         | 4 |
| HO2       | 20387H          | 10              | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.04072191E+02  | 0.02131296E-01  | -0.05308145E-05 | 0.06112269E-09  | -0.02841164E-13 |         |         |         | 2 |
|           | -0.15797270E+03 | 0.03476029E+02  | 0.02979963E+02  | 0.04996697E-01  | -0.03790997E-04 |         |         |         | 3 |
|           | 0.02354192E-07  | -0.08089024E-11 | 0.01762273E+04  | 0.09222724E+02  |                 |         |         |         | 4 |
| HOCN      | 120186H         | 10              | 1C              | 1N              | 1G              | 0250.00 | 4000.00 | 1000.00 | 1 |
|           | 0.05645607E+02  | 0.02298206E-01  | -0.02162629E-05 | -0.12148014E-09 | 0.02238636E-12  |         |         |         | 2 |
|           | -0.03178109E+05 | -0.03590263E+02 | 0.03628292E+02  | 0.05664184E-01  | -0.11702056E-06 |         |         |         | 3 |
|           | -0.02348638E-07 | 0.08016402E-11  | -0.02475925E+05 | 0.07476825E+02  |                 |         |         |         | 4 |
| HONO      | 31787H          | 1N              | 10              | 2               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|           | 0.05486892E+02  | 0.04218064E-01  | -0.16491426E-05 | 0.02971876E-08  | -0.02021148E-12 |         |         |         | 2 |
|           | -0.11268646E+05 | -0.02997002E+02 | 0.02290413E+02  | 0.14099223E-01  | -0.13678717E-04 |         |         |         | 3 |
|           | 0.07498780E-07  | -0.01876905E-10 | -0.10431945E+05 | 0.13280769E+02  |                 |         |         |         | 4 |
| HSI(NH2)2 | 22790SI         | 1H              | 5N              | 2               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.11716773E+02  | 0.05339021E-01  | -0.04667823E-05 | -0.02824087E-08 | 0.05080915E-12  |         |         |         | 2 |
|           | -0.12641686E+04 | -0.03245117E+03 | 0.06289698E+02  | 0.16750596E-01  | -0.15208775E-05 |         |         |         | 3 |
|           | -0.10700650E-07 | 0.05538640E-10  | 0.03154770E+04  | -0.03746008E+02 |                 |         |         |         | 4 |
| HSI(NH2)3 | 22790SI         | 1H              | 7N              | 3               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.16614058E+02  | 0.07395874E-01  | -0.06440009E-05 | -0.03918887E-08 | 0.07045959E-12  |         |         |         | 2 |
|           | -0.03859547E+06 | -0.05865317E+03 | 0.07070983E+02  | 0.02754435E+00  | -0.02603669E-04 |         |         |         | 3 |
|           | -0.01874567E-06 | 0.09778511E-10  | -0.03582658E+06 | -0.08209675E+02 |                 |         |         |         | 4 |
| HSICL     | 121986SI        | 1H              | 1CL             | 1               | G               | 0300.00 | 2000.00 | 1000.00 | 1 |
|           | 0.04900627E+02  | 0.01981752E-01  | -0.03634646E-05 | -0.02285211E-08 | 0.07633527E-12  |         |         |         | 2 |
|           | 0.06914634E+05  | 0.13770041E+01  | 0.03072747E+02  | 0.09057843E-01  | -0.11591338E-04 |         |         |         | 3 |
|           | 0.08310476E-07  | -0.02482999E-10 | 0.07324210E+05  | 0.10334904E+02  |                 |         |         |         | 4 |
| HSIN      | 22790H          | 1SI             | 1N              | 1               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.05746590E+02  | 0.11671186E-02  | -0.13607424E-06 | -0.05908616E-09 | 0.11746961E-13  |         |         |         | 2 |
|           | 0.04484671E+06  | -0.05931788E+02 | 0.04865176E+02  | 0.01775119E-01  | 0.04890869E-05  |         |         |         | 3 |
|           | 0.03922382E-08  | -0.07913276E-11 | 0.04526352E+06  | -0.07134509E+01 |                 |         |         |         | 4 |
| HSINH     | 42489SI         | 1H              | 2N              | 1               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.06493435E+02  | 0.02567980E-01  | -0.03126526E-05 | -0.02577467E-08 | 0.06216479E-12  |         |         |         | 2 |
|           | 0.04035934E+06  | -0.07830112E+02 | 0.03566343E+02  | 0.08446736E-01  | -0.07699952E-05 |         |         |         | 3 |
|           | -0.05270970E-07 | 0.02581065E-10  | 0.04124903E+06  | 0.07780791E+02  |                 |         |         |         | 4 |
| HSINH2    | 42489SI         | 1N              | 1H              | 3               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.06177894E+02  | 0.04689964E-01  | -0.03583293E-05 | -0.04457980E-08 | 0.09379187E-12  |         |         |         | 2 |
|           | 0.10912773E+05  | -0.07006672E+02 | 0.02716144E+02  | 0.12042781E-01  | -0.09827195E-05 |         |         |         | 3 |
|           | -0.07408477E-07 | 0.03789792E-10  | 0.11907715E+05  | 0.11262523E+02  |                 |         |         |         | 4 |

|                 |                 |                 |                 |                 |         |         |         |   |
|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| I*C3H7          | 120186C         | 3H              | 7               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.08063369E+02  | 0.15744876E-01  | -0.05182391E-04 | 0.07477245E-08  | -0.03854422E-12 |         |         |         | 2 |
| 0.05313871E+05  | -0.02192646E+03 | 0.01713299E+02  | 0.02542616E+00  | 0.15808083E-05  |         |         |         | 3 |
| -0.01821286E-06 | 0.08827710E-10  | 0.07535808E+05  | 0.12979008E+02  |                 |         |         |         | 4 |
| ME2GAET         | 62987GA         | 1C              | 4H 11           | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.07174541E+02  | 0.03235532E+00  | 0.14951986E-05  | -0.10482260E-07 | 0.03053961E-10  |         |         |         | 2 |
| -0.06383914E+05 | -0.02026765E+02 | -0.03218207E+02 | 0.06398884E+00  | 0.15545521E-04  |         |         |         | 3 |
| -0.12847095E-06 | 0.09441259E-09  | -0.04451897E+05 | 0.04848091E+03  |                 |         |         |         | 4 |
| MEGAET          | 62987GA         | 1C              | 3H 8            | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.06600990E+02  | 0.02284791E+00  | 0.10133754E-05  | -0.07318045E-07 | 0.02140196E-10  |         |         |         | 2 |
| 0.04071592E+05  | 0.05239051E+01  | -0.08169937E+01 | 0.04554296E+00  | 0.10531326E-04  |         |         |         | 3 |
| -0.09079987E-06 | 0.06700563E-09  | 0.05448005E+05  | 0.03655501E+03  |                 |         |         |         | 4 |
| MEGAET2         | 62987GA         | 1C              | 5H 13           | G               | 0300.00 | 1500.00 | 0600.00 | 1 |
| 0.08123155E+02  | 0.03978908E+00  | 0.01690979E-04  | -0.13084149E-07 | 0.03852598E-10  |         |         |         | 2 |
| -0.08091056E+05 | -0.05039992E+02 | -0.05607498E+02 | 0.08187357E+00  | 0.01920530E-03  |         |         |         | 3 |
| -0.01678978E-05 | 0.12433538E-09  | -0.05546687E+05 | 0.06163371E+03  |                 |         |         |         | 4 |
| N               | 120186N         | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.02450268E+02  | 0.10661458E-03  | -0.07465337E-06 | 0.01879652E-09  | -0.10259839E-14 |         |         |         | 2 |
| 0.05611604E+06  | 0.04448758E+02  | 0.02503071E+02  | -0.02180018E-03 | 0.05420529E-06  |         |         |         | 3 |
| -0.05647560E-09 | 0.02099904E-12  | 0.05609890E+06  | 0.04167566E+02  |                 |         |         |         | 4 |
| N*C3H7          | 120186C         | 3H              | 7               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.07978290E+02  | 0.15761134E-01  | -0.05173243E-04 | 0.07443892E-08  | -0.03824978E-12 |         |         |         | 2 |
| 0.07579402E+05  | -0.01935611E+03 | 0.01922536E+02  | 0.02478927E+00  | 0.01810249E-04  |         |         |         | 3 |
| -0.01783265E-06 | 0.08582996E-10  | 0.09713281E+05  | 0.13992715E+02  |                 |         |         |         | 4 |
| N2              | 121286N         | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.02926640E+02  | 0.14879768E-02  | -0.05684760E-05 | 0.10097038E-09  | -0.06753351E-13 |         |         |         | 2 |
| -0.09227977E+04 | 0.05980528E+02  | 0.03298677E+02  | 0.14082404E-02  | -0.03963222E-04 |         |         |         | 3 |
| 0.05641515E-07  | -0.02444854E-10 | -0.10208999E+04 | 0.03950372E+02  |                 |         |         |         | 4 |
| N2H2            | 121286N         | 2H              | 2               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.03371185E+02  | 0.06039968E-01  | -0.02303853E-04 | 0.04062789E-08  | -0.02713144E-12 |         |         |         | 2 |
| 0.02418172E+06  | 0.04980585E+02  | 0.16179994E+01  | 0.13063122E-01  | -0.01715711E-03 |         |         |         | 3 |
| 0.16056079E-07  | -0.06093638E-10 | 0.02467526E+06  | 0.13794670E+02  |                 |         |         |         | 4 |
| N2H3            | 120186N         | 2H              | 3               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.04441846E+02  | 0.07214270E-01  | -0.02495684E-04 | 0.03920564E-08  | -0.02298949E-12 |         |         |         | 2 |
| 0.16642211E+05  | -0.04275204E+01 | 0.03174203E+02  | 0.04715907E-01  | 0.13348671E-04  |         |         |         | 3 |
| -0.01919684E-06 | 0.07487563E-10  | 0.01727269E+06  | 0.07557224E+02  |                 |         |         |         | 4 |
| N2H4            | 121286N         | 2H              | 4               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.04977317E+02  | 0.09595519E-01  | -0.03547639E-04 | 0.06124299E-08  | -0.04029795E-12 |         |         |         | 2 |
| 0.09341219E+05  | -0.02962989E+02 | 0.06442605E+00  | 0.02749729E+00  | -0.02899451E-03 |         |         |         | 3 |
| 0.01745239E-06  | -0.04422282E-10 | 0.10451917E+05  | 0.02127789E+03  |                 |         |         |         | 4 |
| N2H4(L)         | 90589H          | 4N              | 2               | L               | 0300.00 | 0600.00 | 0450.00 | 1 |
| 0.08890683E+02  | 0.08330343E-01  | 0.04945549E-04  | -0.04909251E-08 | -0.03355824E-10 |         |         |         | 2 |
| 0.03032250E+05  | -0.03871433E+03 | 0.09047444E+02  | 0.09241592E-01  | 0.02263547E-04  |         |         |         | 3 |
| -0.08952247E-07 | 0.14868629E-10  | 0.02970392E+05  | -0.03974033E+03 |                 |         |         |         | 4 |
| N2O             | 121286N         | 2O              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
| 0.04718977E+02  | 0.02873713E-01  | -0.11974958E-05 | 0.02250551E-08  | -0.15753370E-13 |         |         |         | 2 |
| 0.08165811E+05  | -0.16572504E+01 | 0.02543057E+02  | 0.09492193E-01  | -0.09792775E-04 |         |         |         | 3 |
| 0.06263844E-07  | -0.01901825E-10 | 0.08765100E+05  | 0.09511222E+02  |                 |         |         |         | 4 |

|      |                 |                 |                 |                 |                 |         |         |         |   |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| N20+ | 121286N         | 20              | 1E              | -1              | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05398516E+02  | 0.02249478E-01  | -0.09577056E-05 | 0.01823192E-08  | -0.12844222E-13 |         |         |         | 2 |
|      | 0.15848513E+06  | -0.03733146E+02 | 0.03187228E+02  | 0.08350714E-01  | -0.07894548E-04 |         |         |         | 3 |
|      | 0.04597444E-07  | -0.13810748E-11 | 0.15912794E+06  | 0.07779425E+02  |                 |         |         |         | 4 |
| N204 | 121286N         | 20              | 4               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.10482201E+02  | 0.05972272E-01  | -0.02564043E-04 | 0.04916885E-08  | -0.03490969E-12 |         |         |         | 2 |
|      | -0.02849988E+05 | -0.02612289E+03 | 0.03624592E+02  | 0.02474708E+00  | -0.02172874E-03 |         |         |         | 3 |
|      | 0.09927103E-07  | -0.02222817E-10 | -0.09128241E+04 | 0.09457174E+02  |                 |         |         |         | 4 |
| N3   | 121286N         | 3               |                 |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05208505E+02  | 0.02444507E-01  | -0.10389415E-05 | 0.01977416E-08  | -0.13956436E-13 |         |         |         | 2 |
|      | 0.04796178E+06  | -0.03612755E+02 | 0.02882218E+02  | 0.08930338E-01  | -0.08539038E-04 |         |         |         | 3 |
|      | 0.05045585E-07  | -0.15212480E-11 | 0.04863468E+06  | 0.08481757E+02  |                 |         |         |         | 4 |
| NCO  | 121286N         | 1C              | 10              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05012045E+02  | 0.02626773E-01  | -0.11082433E-05 | 0.02093860E-08  | -0.14603470E-13 |         |         |         | 2 |
|      | 0.01737185E+06  | -0.01830075E+02 | 0.02830320E+02  | 0.08871490E-01  | -0.08945636E-04 |         |         |         | 3 |
|      | 0.05876918E-07  | -0.01907734E-10 | 0.01800543E+06  | 0.09498831E+02  |                 |         |         |         | 4 |
| NF   | 121286N         | 1F              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.03862176E+02  | 0.07551806E-02  | -0.03044942E-05 | 0.05874447E-09  | -0.04187479E-13 |         |         |         | 2 |
|      | 0.02867242E+06  | 0.03457232E+02  | 0.02871947E+02  | 0.03312192E-01  | -0.02691158E-04 |         |         |         | 3 |
|      | 0.11219514E-08  | -0.02475130E-11 | 0.02896257E+06  | 0.08640247E+02  |                 |         |         |         | 4 |
| NFO  | 121286N         | 1F              | 10              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05174520E+02  | 0.01938472E-01  | -0.08222701E-05 | 0.15642909E-09  | -0.11044974E-13 |         |         |         | 2 |
|      | -0.09670935E+05 | -0.05352460E+01 | 0.03352307E+02  | 0.07229966E-01  | -0.06951136E-04 |         |         |         | 3 |
|      | 0.03828526E-07  | -0.10235582E-11 | -0.09167035E+05 | 0.08854189E+02  |                 |         |         |         | 4 |
| NFO2 | 121286N         | 1F              | 10              | 2               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.06816857E+02  | 0.03462639E-01  | -0.14922156E-05 | 0.02869665E-08  | -0.02041856E-12 |         |         |         | 2 |
|      | -0.15602619E+05 | -0.09320129E+02 | 0.02447528E+02  | 0.15441095E-01  | -0.13005952E-04 |         |         |         | 3 |
|      | 0.04856383E-07  | -0.06852266E-11 | -0.14393999E+05 | 0.13283604E+02  |                 |         |         |         | 4 |
| NH   | 31387H          | 1N              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02760249E+02  | 0.13753463E-02  | -0.04451914E-05 | 0.07692791E-09  | -0.05017592E-13 |         |         |         | 2 |
|      | 0.04207828E+06  | 0.05857199E+02  | 0.03339758E+02  | 0.12530086E-02  | -0.03491645E-04 |         |         |         | 3 |
|      | 0.04218812E-07  | -0.15576179E-11 | 0.04185047E+06  | 0.02507180E+02  |                 |         |         |         | 4 |
| NH2  | 121686N         | 1H              | 2               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02961311E+02  | 0.02932699E-01  | -0.09063600E-05 | 0.16172575E-09  | -0.12042003E-13 |         |         |         | 2 |
|      | 0.02191976E+06  | 0.05777878E+02  | 0.03432493E+02  | 0.03299540E-01  | -0.06613600E-04 |         |         |         | 3 |
|      | 0.08590947E-07  | -0.03572046E-10 | 0.02177227E+06  | 0.03090110E+02  |                 |         |         |         | 4 |
| NH3  | 121386N         | 1H              | 3               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02461904E+02  | 0.06059166E-01  | -0.02004976E-04 | 0.03136003E-08  | -0.01938317E-12 |         |         |         | 2 |
|      | -0.06493269E+05 | 0.07472097E+02  | 0.02204351E+02  | 0.10114765E-01  | -0.14652648E-04 |         |         |         | 3 |
|      | 0.14472350E-07  | -0.05328509E-10 | -0.06525488E+05 | 0.08127138E+02  |                 |         |         |         | 4 |
| NNH  | 120186N         | 2H              | 1               |                 | G               | 0250.00 | 4000.00 | 1000.00 | 1 |
|      | 0.04415342E+02  | 0.16143879E-02  | -0.16328943E-06 | -0.08559846E-09 | 0.16147909E-13  |         |         |         | 2 |
|      | 0.02788029E+06  | 0.09042888E+01  | 0.03501344E+02  | 0.02053586E-01  | 0.07170409E-05  |         |         |         | 3 |
|      | 0.04921348E-08  | -0.09671170E-11 | 0.02833347E+06  | 0.06391837E+02  |                 |         |         |         | 4 |
| NO   | 121286N         | 10              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.03245435E+02  | 0.12691383E-02  | -0.05015890E-05 | 0.09169283E-09  | -0.06275419E-13 |         |         |         | 2 |
|      | 0.09800840E+05  | 0.06417293E+02  | 0.03376541E+02  | 0.12530634E-02  | -0.03302750E-04 |         |         |         | 3 |
|      | 0.05217810E-07  | -0.02446262E-10 | 0.09817961E+05  | 0.05829590E+02  |                 |         |         |         | 4 |

|      |                 |                 |                |                 |                |         |         |         |   |
|------|-----------------|-----------------|----------------|-----------------|----------------|---------|---------|---------|---|
| NO+  | 121286N         | 10              | 1E             | -1              | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02914888E+02  | 0.14993349E-02  | 0.05727972E-05 | 0.10177767E-09  | 0.06825390E-13 |         |         |         | 2 |
|      | 0.11818688E+06  | 0.06844346E+02  | 0.03297349E+02 | 0.14228899E-02  | 0.04007441E-04 |         |         |         | 3 |
|      | 0.05670551E-07  | 0.02446971E-10  | 0.11808338E+06 | 0.04749948E+02  |                |         |         |         | 4 |
| N02  | 121286N         | 10              | 2              |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.04682859E+02  | 0.02462429E-01  | 0.10422585E-05 | 0.01976902E-08  | 0.13917168E-13 |         |         |         | 2 |
|      | 0.02261292E+05  | 0.09885985E+01  | 0.02670600E+02 | 0.07838500E-01  | 0.08063864E-04 |         |         |         | 3 |
|      | 0.06161714E-07  | 0.02320150E-10  | 0.02896290E+05 | 0.11612071E+02  |                |         |         |         | 4 |
| N02- | 121286N         | 10              | 2E             | 1               | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05043114E+02  | 0.02166427E-01  | 0.09455454E-05 | 0.01816313E-08  | 0.12383945E-13 |         |         |         | 2 |
|      | -0.02621553E+06 | -0.14459051E+01 | 0.02448586E+02 | 0.08982507E-01  | 0.07853431E-04 |         |         |         | 3 |
|      | 0.03927276E-07  | 0.10716939E-11  | 0.02545097E+06 | 0.12130600E+02  |                |         |         |         | 4 |
| N03  | 121286N         | 10              | 3              |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.07120307E+02  | 0.03246228E-01  | 0.14316134E-05 | 0.02797053E-08  | 0.02013007E-12 |         |         |         | 2 |
|      | 0.05864479E+05  | 0.12137301E+02  | 0.12210763E+01 | 0.01878797E+00  | 0.13443212E-04 |         |         |         | 3 |
|      | 0.12746013E-08  | 0.13540601E-11  | 0.07473144E+05 | 0.01840202E+03  |                |         |         |         | 4 |
| 0    | 1201860         | 1               |                |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02542059E+02  | 0.02755061E-03  | 0.03102803E-07 | 0.04551067E-10  | 0.04368051E-14 |         |         |         | 2 |
|      | 0.02923080E+06  | 0.04920308E+02  | 0.02946428E+02 | -0.16381665E-02 | 0.02421031E-04 |         |         |         | 3 |
|      | -0.16028431E-08 | 0.03890696E-11  | 0.02914764E+06 | 0.02963995E+02  |                |         |         |         | 4 |
| 0+   | 1212860         | 1E              | -1             |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02501869E+02  | 0.06107262E-04  | 0.07324307E-07 | -0.03438353E-10 | 0.05506407E-14 |         |         |         | 2 |
|      | 0.01879552E+07  | 0.04372826E+02  | 0.02499272E+02 | 0.05820598E-04  | 0.11209219E-07 |         |         |         | 3 |
|      | 0.08232108E-10  | 0.01916378E-13  | 0.01879556E+07 | 0.04384825E+02  |                |         |         |         | 4 |
| 0-   | 905890          | 1E              | 1              |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02559580E+02  | 0.07147887E-03  | 0.03301804E-06 | -0.06660944E-10 | 0.04900726E-14 |         |         |         | 2 |
|      | 0.11489346E+05  | 0.04426186E+02  | 0.02747263E+02 | -0.05724860E-02 | 0.02712548E-05 |         |         |         | 3 |
|      | 0.02691511E-08  | 0.02002357E-11  | 0.11443947E+05 | 0.03469852E+02  |                |         |         |         | 4 |
| 02   | 1213860         | 2               |                |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.03697578E+02  | 0.06135197E-02  | 0.12588420E-06 | 0.01775281E-09  | 0.11364354E-14 |         |         |         | 2 |
|      | -0.12339301E+04 | 0.03189165E+02  | 0.03212936E+02 | 0.11274864E-02  | 0.05756150E-05 |         |         |         | 3 |
|      | 0.13138773E-08  | 0.08768554E-11  | 0.10052490E+04 | 0.06034737E+02  |                |         |         |         | 4 |
| 02-  | 1212860         | 2E              | 1              |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.03883013E+02  | 0.07407872E-02  | 0.02961776E-05 | 0.05724304E-09  | 0.04086547E-13 |         |         |         | 2 |
|      | -0.07121644E+05 | 0.02658211E+02  | 0.02872291E+02 | 0.03359716E-01  | 0.02664886E-04 |         |         |         | 3 |
|      | 0.09807524E-08  | 0.16709571E-12  | 0.06829094E+05 | 0.07938372E+02  |                |         |         |         | 4 |
| 03   | 1212860         | 3               |                |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.05429371E+02  | 0.01820380E-01  | 0.07705607E-05 | 0.14992929E-09  | 0.10755629E-13 |         |         |         | 2 |
|      | 0.15235267E+05  | 0.03266386E+02  | 0.02462608E+02 | 0.09582781E-01  | 0.07087359E-04 |         |         |         | 3 |
|      | 0.13633683E-08  | 0.02969647E-11  | 0.16061522E+05 | 0.12141870E+02  |                |         |         |         | 4 |
| OH   | 1212860         | 1H              | 1              |                 | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02882730E+02  | 0.10139743E-02  | 0.02276877E-05 | 0.02174683E-09  | 0.05126305E-14 |         |         |         | 2 |
|      | 0.03886888E+05  | 0.05595712E+02  | 0.03637266E+02 | 0.01850910E-02  | 0.16761646E-05 |         |         |         | 3 |
|      | 0.02387202E-07  | 0.08431442E-11  | 0.03606781E+05 | 0.13588605E+01  |                |         |         |         | 4 |
| OH+  | 1212860         | 1H              | 1E             | -1              | G              | 0300.00 | 5000.00 | 1000.00 | 1 |
|      | 0.02719058E+02  | 0.15085714E-02  | 0.05029369E-05 | 0.08261951E-09  | 0.04947452E-13 |         |         |         | 2 |
|      | 0.15763414E+06  | 0.06234536E+02  | 0.03326978E+02 | 0.13457859E-02  | 0.03777167E-04 |         |         |         | 3 |
|      | 0.04687749E-07  | 0.01780982E-10  | 0.15740294E+06 | 0.02744042E+02  |                |         |         |         | 4 |

|            |                 |                 |                 |                 |                 |         |         |         |   |
|------------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| OH-        | 1212860         | 1H              | 1E              | 1               | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.02846204E+02  | 0.10418347E-02  | -0.02416850E-05 | 0.02483215E-09  | -0.07775605E-14 |         |         |         | 2 |
|            | -0.01807280E+06 | 0.04422712E+02  | 0.03390037E+02  | 0.07922381E-02  | -0.01943429E-04 |         |         |         | 3 |
|            | 0.02001769E-07  | -0.05702087E-11 | -0.01830493E+06 | 0.12498923E+01  |                 |         |         |         | 4 |
| S          | 121286S         | 1               |                 |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.02902148E+02  | -0.05484546E-02 | 0.02764576E-05  | -0.05017114E-09 | 0.03150684E-13  |         |         |         | 2 |
|            | 0.03249423E+06  | 0.03838471E+02  | 0.03187329E+02  | -0.15957763E-02 | 0.02005531E-04  |         |         |         | 3 |
|            | -0.15070814E-08 | 0.04931282E-11  | 0.03242259E+06  | 0.02414441E+02  |                 |         |         |         | 4 |
| S(L)       | 120186S         | 1               |                 |                 | L               | 0388.36 | 2000.00 | 1000.00 | 1 |
|            | 0.03603667E+02  | 0.09903341E-02  | -0.10114410E-05 | 0.04053632E-08  | -0.05667913E-12 |         |         |         | 2 |
|            | -0.08453839E+04 | -0.16344708E+02 | -0.12706310E+02 | 0.09072521E+00  | -0.01695178E-02 |         |         |         | 3 |
|            | 0.13070636E-06  | -0.03527615E-09 | 0.12346069E+04  | 0.05621016E+03  |                 |         |         |         | 4 |
| S(S)       | 120186S         | 1               |                 |                 | S               | 0300.00 | 0388.36 | 1000.00 | 1 |
|            | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 2 |
|            | 0.00000000E+00  | 0.00000000E+00  | -0.05063702E+02 | 0.02881935E-01  | -0.02133020E-03 |         |         |         | 3 |
|            | 0.08478786E-05  | -0.01734496E-07 | 0.07148263E+04  | 0.02871407E+03  |                 |         |         |         | 4 |
| S+         | 121286S         | 1E              | -1              |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.02404600E+02  | 0.02410908E-02  | -0.02041779E-05 | 0.06592945E-09  | -0.05756939E-13 |         |         |         | 2 |
|            | 0.15352225E+06  | 0.05924256E+02  | 0.02366100E+02  | 0.09130767E-02  | -0.02140283E-04 |         |         |         | 3 |
|            | 0.02076177E-07  | -0.07133859E-11 | 0.15350910E+06  | 0.05993094E+02  |                 |         |         |         | 4 |
| S-TRIAZINE | 41687C          | 3N              | 3H              | 3               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.13036170E+02  | 0.07711820E-01  | -0.07724374E-05 | -0.04385191E-08 | 0.08298992E-12  |         |         |         | 2 |
|            | 0.02251663E+06  | -0.04777676E+03 | 0.04493492E+01  | 0.02728306E+00  | 0.02309304E-04  |         |         |         | 3 |
|            | -0.14968443E-07 | 0.04546753E-10  | 0.02703032E+06  | 0.02178518E+03  |                 |         |         |         | 4 |
| S2         | 121386S         | 1               |                 |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.03904443E+02  | 0.06925733E-02  | -0.12330970E-06 | 0.08783809E-11  | 0.13746621E-14  |         |         |         | 2 |
|            | 0.14256933E+05  | 0.04956834E+02  | 0.03157672E+02  | 0.03099480E-01  | -0.15607465E-05 |         |         |         | 3 |
|            | -0.13578905E-08 | 0.11374435E-11  | 0.14391873E+05  | 0.08596062E+02  |                 |         |         |         | 4 |
| SH         | 121286S         | 1H              | 1               |                 | G               | 0300.00 | 5000.00 | 1000.00 | 1 |
|            | 0.03053810E+02  | 0.12588843E-02  | -0.04249169E-05 | 0.06929591E-09  | -0.04281691E-13 |         |         |         | 2 |
|            | 0.15882250E+05  | 0.05973551E+02  | 0.04133326E+02  | -0.03787893E-02 | -0.02777854E-04 |         |         |         | 3 |
|            | 0.05370112E-07  | -0.02394006E-10 | 0.15558623E+05  | 0.16115348E+00  |                 |         |         |         | 4 |
| SI         | 32989SI         | 1               |                 |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.02775845E+02  | -0.06213257E-02 | 0.04843696E-05  | -0.12756146E-09 | 0.11344818E-13  |         |         |         | 2 |
|            | 0.05339790E+06  | 0.04543298E+02  | 0.03113515E+02  | -0.02330991E-01 | 0.03518530E-04  |         |         |         | 3 |
|            | -0.02417573E-07 | 0.06391902E-11  | 0.05335061E+06  | 0.03009718E+02  |                 |         |         |         | 4 |
| SI(L)      | 90589SI         | 1               |                 |                 | L               | 0300.00 | 4500.00 | 1000.00 | 1 |
|            | 0.03271263E+02  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 2 |
|            | 0.04855057E+05  | -0.13290542E+02 | 0.03271263E+02  | 0.00000000E+00  | 0.00000000E+00  |         |         |         | 3 |
|            | 0.00000000E+00  | 0.00000000E+00  | 0.04855058E+05  | -0.13290542E+02 |                 |         |         |         | 4 |
| SI(NH2)3   | 42489SI         | 1N              | 3H              | 6               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|            | 0.14065501E+02  | 0.07581744E-01  | -0.05168510E-05 | -0.06743626E-08 | 0.13979258E-12  |         |         |         | 2 |
|            | -0.14144028E+05 | -0.04063873E+03 | 0.07598413E+02  | 0.02435266E+00  | -0.04296202E-04 |         |         |         | 3 |
|            | -0.01756006E-06 | 0.10501017E-10  | -0.12653434E+05 | -0.07808647E+02 |                 |         |         |         | 4 |
| SI(NH2)4   | 22790SI         | 1N              | 4H              | 8               | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|            | 0.02032107E+03  | 0.08289798E-01  | -0.07077612E-05 | -0.04340724E-08 | 0.07747068E-12  |         |         |         | 2 |
|            | -0.05389855E+06 | -0.07730464E+03 | 0.08454529E+02  | 0.03465772E+00  | -0.04266782E-04 |         |         |         | 3 |
|            | -0.02495363E-06 | 0.13654663E-10  | -0.05061518E+06 | -0.15143013E+02 |                 |         |         |         | 4 |



|                 |                 |                 |                 |                 |         |         |   |
|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---|
| SI(S)           | 90589SI         | 1               | S               | 0300.00         | 2500.00 | 1000.00 | 1 |
| 0.02530275E+02  | 0.08522433E-02  | -0.03223468E-05 | 0.12808208E-09  | -0.01850849E-12 |         |         | 2 |
| -0.08395197E+04 | -0.12514782E+02 | 0.05746418E+01  | 0.10264855E-01  | -0.01775345E-03 |         |         | 3 |
| 0.14575000E-07  | -0.04491292E-10 | -0.04969951E+04 | -0.03400242E+02 |                 |         |         | 4 |
| SI2             | 90589SI         | 2               | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
| 0.04232196E+02  | 0.04315355E-02  | -0.02964833E-05 | 0.09823294E-09  | -0.12962688E-13 |         |         | 2 |
| 0.06964651E+06  | 0.03308527E+02  | 0.02993750E+02  | 0.06053689E-01  | -0.10158575E-04 |         |         | 3 |
| 0.07909737E-07  | -0.02346083E-10 | 0.06987498E+06  | 0.09151741E+02  |                 |         |         | 4 |
| SI2C            | 112989C         | 1SI 2           | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
| 0.06334110E+02  | 0.12102520E-02  | -0.06798289E-05 | 0.02244432E-08  | -0.02280177E-12 |         |         | 2 |
| 0.06227189E+06  | -0.07770097E+02 | 0.04157246E+02  | 0.07031825E-01  | -0.07263033E-04 |         |         | 3 |
| 0.04633583E-07  | -0.14934475E-11 | 0.06292421E+06  | 0.03635125E+02  |                 |         |         | 4 |
| SI2F6           | 42489SI         | 2F 6            | G               | 0300.00         | 3000.00 | 1000.00 | 1 |
| 0.01830047E+03  | 0.02868752E-01  | -0.04545576E-05 | -0.02497900E-08 | 0.06630658E-12  |         |         | 2 |
| -0.02928185E+07 | -0.05760425E+03 | 0.09998134E+02  | 0.02170313E+00  | -0.03875091E-04 |         |         | 3 |
| -0.16702523E-07 | 0.09407529E-10  | -0.02905482E+07 | -0.14228863E+02 |                 |         |         | 4 |
| SI2H2           | 90589SI         | 2H 2            | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
| 0.05778180E+02  | 0.04070596E-01  | -0.04259125E-05 | -0.07920228E-08 | 0.02379752E-11  |         |         | 2 |
| 0.03980520E+06  | -0.05392375E+02 | 0.16247229E+01  | 0.14871029E-01  | -0.08707160E-04 |         |         | 3 |
| -0.01699554E-09 | 0.10972211E-11  | 0.04095325E+06  | 0.16165730E+02  |                 |         |         | 4 |
| SI2H3           | 90589SI         | 2H 3            | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
| 0.07257627E+02  | 0.05123859E-01  | -0.07633465E-05 | -0.06662471E-08 | 0.02053052E-11  |         |         | 2 |
| 0.05062055E+06  | -0.10314127E+02 | 0.03335404E+02  | 0.02155614E+00  | -0.02933937E-03 |         |         | 3 |
| 0.02287784E-06  | -0.07272827E-10 | 0.05146157E+06  | 0.08656853E+02  |                 |         |         | 4 |
| SI2H5           | 90589SI         | 2H 5            | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
| 0.08451010E+02  | 0.09286371E-01  | -0.10911831E-05 | -0.14423673E-08 | 0.04250824E-11  |         |         | 2 |
| 0.02472718E+06  | -0.01710331E+03 | 0.15788481E+01  | 0.03549382E+00  | -0.04267511E-03 |         |         | 3 |
| 0.03059177E-06  | -0.09360425E-10 | 0.02630549E+06  | 0.16720734E+02  |                 |         |         | 4 |
| SI2H6           | 90589SI         | 2H 6            | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
| 0.08882090E+02  | 0.11513955E-01  | -0.12162159E-05 | -0.01905085E-07 | 0.05542379E-11  |         |         | 2 |
| 0.05967241E+05  | -0.02265611E+03 | 0.05301921E+01  | 0.04184055E+00  | -0.04685249E-03 |         |         | 3 |
| 0.03179525E-06  | -0.09484526E-10 | 0.07950597E+05  | 0.01880453E+03  |                 |         |         | 4 |
| SI3             | 32989SI         | 3               | G               | 0300.00         | 4000.00 | 1000.00 | 1 |
| 0.07021584E+02  | 0.06981538E-02  | -0.04818729E-05 | 0.01720754E-08  | -0.01927024E-12 |         |         | 2 |
| 0.07429956E+06  | -0.08179232E+02 | 0.05312161E+02  | 0.05920180E-01  | -0.05075224E-04 |         |         | 3 |
| 0.05303866E-08  | 0.07031630E-11  | 0.07469501E+06  | 0.04036452E+01  |                 |         |         | 4 |
| SI3H8           | 90589SI         | 3H 8            | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
| 0.13422770E+02  | 0.15636323E-01  | -0.01936565E-04 | -0.02388329E-07 | 0.07120030E-11  |         |         | 2 |
| 0.09165887E+05  | -0.04163000E+03 | 0.06319791E+01  | 0.06412995E+00  | -0.07772444E-03 |         |         | 3 |
| 0.05486969E-06  | -0.16460971E-10 | 0.12092580E+05  | 0.02133318E+03  |                 |         |         | 4 |
| SI3N4(A)        | 42589N          | 4SI 3           | S               | 0300.00         | 3000.00 | 1000.00 | 1 |
| 0.09667453E+02  | 0.11927212E-01  | -0.01709281E-04 | -0.10846074E-08 | 0.02713018E-11  |         |         | 2 |
| -0.09324734E+06 | -0.04556492E+03 | 0.06631384E+02  | 0.02293928E+00  | -0.02152875E-03 |         |         | 3 |
| 0.01766237E-06  | -0.06632214E-10 | -0.09241684E+06 | -0.03021795E+03 |                 |         |         | 4 |
| SIC             | 112989C         | 1SI 1           | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
| 0.05024270E+02  | -0.04920894E-02 | 0.03109315E-05  | -0.06901344E-09 | 0.05215735E-13  |         |         | 2 |
| 0.08531026E+06  | -0.02478798E+02 | 0.02427812E+02  | 0.09551934E-01  | -0.02796633E-04 |         |         | 3 |
| -0.13600122E-07 | 0.09196322E-10  | 0.08546512E+06  | 0.09179253E+02  |                 |         |         | 4 |

|           |                 |                 |                 |                 |                 |         |         |   |
|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---|
| SIC(B)    | 112989C         | 1SI             | 1               | S               | 0300.00         | 4000.00 | 1000.00 | 1 |
|           | 0.03548056E+02  | 0.03636817E-01  | -0.01734872E-04 | 0.03912869E-08  | -0.03337952E-12 |         |         | 2 |
|           | -0.10188585E+05 | -0.01967253E+03 | -0.03551395E+01 | 0.15998806E-01  | -0.13933268E-04 |         |         | 3 |
|           | 0.03314914E-07  | 0.07825957E-11  | -0.09294352E+05 | -0.15153885E+00 |                 |         |         | 4 |
| SIC2      | 112989C         | 2SI             | 1               | G               | 0300.00         | 5000.00 | 1000.00 | 1 |
|           | 0.05753725E+02  | 0.02067546E-01  | -0.11325346E-05 | 0.03106456E-08  | -0.02799936E-12 |         |         | 2 |
|           | 0.07200461E+06  | -0.05294926E+02 | 0.03647724E+02  | 0.08765100E-01  | -0.10798686E-04 |         |         | 3 |
|           | 0.07974287E-07  | -0.02617042E-10 | 0.07258578E+06  | 0.05481049E+02  |                 |         |         | 4 |
| SICL      | 121986SI        | 1CL             | 1               | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
|           | 0.04258459E+02  | 0.04020317E-02  | -0.02888145E-05 | 0.10097771E-09  | -0.14110117E-13 |         |         | 2 |
|           | 0.01775613E+06  | 0.04134521E+02  | 0.03096406E+02  | 0.05738623E-01  | -0.09740903E-04 |         |         | 3 |
|           | 0.07643597E-07  | -0.02279178E-10 | 0.01796794E+06  | 0.09603212E+02  |                 |         |         | 4 |
| SICL2     | 121986SI        | 1CL             | 2               | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
|           | 0.06491204E+02  | 0.08242384E-02  | -0.05767737E-05 | 0.01972405E-08  | -0.02713757E-12 |         |         | 2 |
|           | -0.02232408E+06 | -0.03570531E+02 | 0.03826666E+02  | 0.13082964E-01  | -0.02234087E-03 |         |         | 3 |
|           | 0.01760741E-06  | -0.05267404E-10 | -0.02183869E+06 | 0.08965448E+02  |                 |         |         | 4 |
| SICL2H2   | 121986SI        | 1H              | 2CL 2           | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
|           | 0.07727079E+02  | 0.05034188E-01  | -0.10957459E-05 | -0.04419587E-08 | 0.16311241E-12  |         |         | 2 |
|           | -0.04028605E+06 | -0.11708156E+02 | 0.11002086E+01  | 0.03262361E+00  | -0.04691994E-03 |         |         | 3 |
|           | 0.03494565E-06  | -0.10362847E-10 | -0.03892086E+06 | 0.02022693E+03  |                 |         |         | 4 |
| SICL3     | 121986SI        | 1CL             | 3               | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
|           | 0.09098097E+02  | 0.14053526E-02  | -0.09317005E-05 | 0.02982296E-08  | -0.03822010E-12 |         |         | 2 |
|           | -0.04140193E+06 | -0.14550117E+02 | 0.04485690E+02  | 0.02241754E+00  | -0.03794196E-03 |         |         | 3 |
|           | 0.02973183E-06  | -0.08861335E-10 | -0.04055264E+06 | 0.07198771E+02  |                 |         |         | 4 |
| SICL3H    | 121986SI        | 1H              | 1CL 3           | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
|           | 0.09663121E+02  | 0.03563367E-01  | -0.12149114E-05 | -0.16090094E-10 | 0.05641710E-12  |         |         | 2 |
|           | -0.06295557E+06 | -0.01894777E+03 | 0.02883769E+02  | 0.03308240E+00  | -0.05169241E-03 |         |         | 3 |
|           | 0.03949918E-06  | -0.11721043E-10 | -0.06163323E+06 | 0.13374664E+02  |                 |         |         | 4 |
| SICL4     | 121986SI        | 1CL             | 4               | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
|           | 0.11709377E+02  | 0.01972091E-01  | -0.12690771E-05 | 0.03900188E-08  | -0.04756468E-12 |         |         | 2 |
|           | -0.08347808E+06 | -0.02791153E+03 | 0.05252110E+02  | 0.03122067E+00  | -0.05254593E-03 |         |         | 3 |
|           | 0.04102707E-06  | -0.12199071E-10 | -0.08228177E+06 | 0.02575727E+02  |                 |         |         | 4 |
| SICLH3    | 121986SI        | 1H              | 3CL 1           | G               | 0300.00         | 2000.00 | 1000.00 | 1 |
|           | 0.05964237E+02  | 0.06278087E-01  | -0.08205634E-05 | -0.09280558E-08 | 0.02796642E-11  |         |         | 2 |
|           | -0.01854309E+06 | -0.06395305E+02 | 0.05057173E+01  | 0.02703377E+00  | -0.03301474E-03 |         |         | 3 |
|           | 0.02302732E-06  | -0.06778703E-10 | -0.01730819E+06 | 0.02043167E+03  |                 |         |         | 4 |
| SIF       | 42489SI         | 1F              | 1               | G               | 0300.00         | 3000.00 | 1000.00 | 1 |
|           | 0.04120066E+02  | 0.03548820E-02  | -0.07200222E-06 | -0.02190434E-09 | 0.06764591E-13  |         |         | 2 |
|           | -0.07561378E+05 | 0.02784246E+02  | 0.03144947E+02  | 0.02588557E-01  | -0.05795912E-05 |         |         | 3 |
|           | -0.01807278E-07 | 0.10411718E-11  | -0.07294439E+05 | 0.07876774E+02  |                 |         |         | 4 |
| SIF(NH2)2 | 22790SI         | 1F              | 1N 2H 4G        | 0300.00         | 4000.00         | 1000.00 | 1       |   |
|           | 0.12879436E+02  | 0.04598535E-01  | -0.04004440E-05 | -0.02374189E-08 | 0.04255211E-12  |         |         | 2 |
|           | -0.05238278E+06 | -0.03653418E+03 | 0.07210094E+02  | 0.01764697E+00  | -0.02542059E-04 |         |         | 3 |
|           | -0.12422138E-07 | 0.06989787E-10  | -0.05086706E+06 | -0.07024622E+02 |                 |         |         | 4 |
| SIF(NH2)3 | 42489SI         | 1N              | 3H 6F 1G        | 0300.00         | 3000.00         | 1000.00 | 1       |   |
|           | 0.16111795E+02  | 0.08329222E-01  | -0.06023787E-05 | -0.07470125E-08 | 0.15707311E-12  |         |         | 2 |
|           | -0.09137007E+06 | -0.05098123E+03 | 0.08388268E+02  | 0.02746622E+00  | -0.04455674E-04 |         |         | 3 |
|           | -0.01955732E-06 | 0.11407210E-10  | -0.08947806E+06 | -0.11381777E+02 |                 |         |         | 4 |



|                 |                 |                 |                 |                 |         |         |         |         |
|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---------|
| SIF2            | 42489SI         | 1F              | 2               | G               | 0300.00 | 3000.00 | 1000.00 | 1       |
| 0.06142470E+02  | 0.07807974E-02  | -0.13393119E-06 | -0.06264839E-09 | 0.01725138E-12  |         |         |         | 2       |
| -0.07744042E+06 | -0.04712327E+02 | 0.03845345E+02  | 0.06038465E-01  | -0.11677323E-05 |         |         |         | 3       |
| -0.04579553E-07 | 0.02607414E-10  | -0.07681633E+06 | 0.07272983E+02  |                 |         |         |         | 4       |
| SIF2(NH2)2      | 42489SI         | 1N              | 2H              | 4F              | 2G      | 0300.00 | 3000.00 | 1000.00 |
| 0.14414775E+02  | 0.06110646E-01  | -0.04871145E-05 | -0.05455935E-08 | 0.11727140E-12  |         |         |         | 1       |
| -0.12927572E+06 | -0.04308682E+03 | 0.07634268E+02  | 0.02315843E+00  | -0.04193827E-04 |         |         |         | 2       |
| -0.01715350E-06 | 0.10164619E-10  | -0.12764102E+06 | -0.08419031E+02 |                 |         |         |         | 3       |
| SIF2N           | 42489SI         | 1N              | 1F              | 2               | G       | 0300.00 | 3000.00 | 1000.00 |
| 0.08687337E+02  | 0.11934885E-02  | -0.01992660E-05 | -0.09951333E-09 | 0.02704383E-12  |         |         |         | 1       |
| -0.03463832E+06 | -0.14940526E+02 | 0.05102583E+02  | 0.09456606E-01  | -0.01819383E-04 |         |         |         | 2       |
| -0.07309616E-07 | 0.04178902E-10  | -0.03367293E+06 | 0.03734423E+02  |                 |         |         |         | 3       |
| SIF2NH2         | 42489SI         | 1N              | 1F              | 2H              | 2G      | 0300.00 | 3000.00 | 1000.00 |
| 0.09872415E+02  | 0.03722112E-01  | -0.03271338E-05 | -0.03321674E-08 | 0.07293692E-12  |         |         |         | 1       |
| -0.08751628E+06 | -0.01899095E+03 | 0.05890444E+02  | 0.12851282E-01  | -0.01863556E-04 |         |         |         | 2       |
| -0.08718963E-07 | 0.04848951E-10  | -0.08644527E+06 | 0.01756162E+02  |                 |         |         |         | 3       |
| SIF3            | 42489SI         | 1F              | 3               | G               | 0300.00 | 3000.00 | 1000.00 | 4       |
| 0.08524790E+02  | 0.13237924E-02  | -0.02104278E-05 | -0.11495040E-09 | 0.03055301E-12  |         |         |         | 1       |
| -0.12235223E+06 | -0.15502343E+02 | 0.04662868E+02  | 0.10087878E-01  | -0.01805544E-04 |         |         |         | 2       |
| -0.07769299E-07 | 0.04377851E-10  | -0.12129652E+06 | 0.04672966E+02  |                 |         |         |         | 3       |
| SIF3NH          | 42489SI         | 1N              | 1F              | 3H              | 1G      | 0300.00 | 3000.00 | 1000.00 |
| 0.11637665E+02  | 0.02880768E-01  | -0.03357310E-05 | -0.02584594E-08 | 0.06162371E-12  |         |         |         | 1       |
| -0.12958909E+06 | -0.02590717E+03 | 0.06013822E+02  | 0.15977294E-01  | -0.02791466E-04 |         |         |         | 2       |
| -0.12141200E-07 | 0.06927415E-10  | -0.12809741E+06 | 0.03316770E+02  |                 |         |         |         | 3       |
| SIF3NH2         | 42489SI         | 1N              | 1F              | 3H              | 2G      | 0300.00 | 3000.00 | 1000.00 |
| 0.12109636E+02  | 0.04383282E-01  | -0.04142245E-05 | -0.03989090E-08 | 0.08958954E-12  |         |         |         | 1       |
| -0.16417679E+06 | -0.03046928E+03 | 0.06229403E+02  | 0.01778015E+00  | -0.02612304E-04 |         |         |         | 2       |
| -0.12672434E-07 | 0.07044556E-10  | -0.16258489E+06 | 0.02045440E+01  |                 |         |         |         | 3       |
| SIF3NHSIH3      | 42489SI         | 2N              | 1H              | 4F              | 3G      | 0300.00 | 3000.00 | 1000.00 |
| 0.16699406E+02  | 0.07789784E-01  | -0.08110570E-05 | -0.07650199E-08 | 0.01773956E-11  |         |         |         | 1       |
| -0.16734123E+06 | -0.05080007E+03 | 0.06216046E+02  | 0.02939330E+00  | -0.02717745E-04 |         |         |         | 2       |
| -0.01982877E-06 | 0.10027676E-10  | -0.16422818E+06 | 0.04858261E+02  |                 |         |         |         | 3       |
| SIF3NSIH3       | 42489SI         | 2N              | 1H              | 3F              | 3G      | 0300.00 | 3000.00 | 1000.00 |
| 0.15991462E+02  | 0.06371085E-01  | -0.07256823E-05 | -0.06292690E-08 | 0.14951566E-12  |         |         |         | 1       |
| -0.13311576E+06 | -0.04495265E+03 | 0.06404371E+02  | 0.02601982E+00  | -0.02491543E-04 |         |         |         | 2       |
| -0.01769542E-06 | 0.08919883E-10  | -0.13025197E+06 | 0.06002945E+02  |                 |         |         |         | 3       |
| SIF4            | 41389F          | 4SI             | 1               | G               | 0300.00 | 2000.00 | 1000.00 | 4       |
| 0.09985301E+02  | 0.03532637E-01  | -0.11973776E-05 | -0.10365486E-09 | 0.08661585E-12  |         |         |         | 1       |
| -0.01977199E+07 | -0.02472643E+03 | 0.02147416E+02  | 0.03402219E+00  | -0.04756873E-03 |         |         |         | 2       |
| 0.03252196E-06  | -0.08819304E-10 | -0.01960449E+07 | 0.13463150E+02  |                 |         |         |         | 3       |
| SIFH3           | 42489SI         | 1F              | 1H              | 3               | G       | 0300.00 | 3000.00 | 1000.00 |
| 0.06799678E+02  | 0.04747086E-01  | -0.04767066E-05 | -0.04814665E-08 | 0.11077613E-12  |         |         |         | 1       |
| -0.04577024E+06 | -0.12614326E+02 | 0.02032189E+02  | 0.13413632E-01  | -0.02806381E-05 |         |         |         | 2       |
| -0.07803291E-07 | 0.03337474E-10  | -0.04421627E+06 | 0.13187677E+02  |                 |         |         |         | 3       |
| SIFNH           | 42489SI         | 1N              | 1F              | 1H              | 1G      | 0300.00 | 3000.00 | 1000.00 |
| 0.07163298E+02  | 0.15213245E-02  | -0.15363371E-06 | -0.11959331E-09 | 0.02684099E-12  |         |         |         | 1       |
| -0.09065496E+05 | -0.06764144E+02 | 0.05390691E+02  | 0.06071319E-01  | -0.13594903E-05 |         |         |         | 2       |
| -0.04267435E-07 | 0.02603153E-10  | -0.08644237E+05 | 0.02272064E+02  |                 |         |         |         | 3       |

|           |                 |                 |                 |                 |                 |         |         |         |   |
|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| SIFNH2    | 22790F          | 1SI             | 1N              | 1H              | 2G              | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.08017582E+02  | 0.03209103E-01  | -0.03361364E-05 | -0.01796536E-08 | 0.03385552E-12  |         |         |         | 2 |
|           | -0.04313426E+06 | -0.14870236E+02 | 0.04214050E+02  | 0.11054231E-01  | -0.10147254E-05 |         |         |         | 3 |
|           | -0.07143728E-07 | 0.03634922E-10  | -0.04200629E+06 | 0.05318889E+02  |                 |         |         |         | 4 |
| SIH       | 121986SI        | 1H              | 1               |                 | G               | 0300.00 | 2000.00 | 1000.00 | 1 |
|           | 0.03110430E+02  | 0.10949460E-02  | 0.02898628E-06  | -0.02745104E-08 | 0.07051799E-12  |         |         |         | 2 |
|           | 0.04516897E+06  | 0.04193487E+02  | 0.03836009E+02  | -0.02702656E-01 | 0.06849070E-04  |         |         |         | 3 |
|           | -0.05424184E-07 | 0.14721313E-11  | 0.04507593E+06  | 0.09350778E+01  |                 |         |         |         | 4 |
| SIH2      | 42489SI         | 1H              | 2               |                 | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.04142390E+02  | 0.02150191E-01  | -0.02190730E-05 | -0.02073725E-08 | 0.04741018E-12  |         |         |         | 2 |
|           | 0.03110483E+06  | 0.02930745E+01  | 0.03475092E+02  | 0.02139338E-01  | 0.07672305E-05  |         |         |         | 3 |
|           | 0.05217668E-08  | -0.09898824E-11 | 0.03147397E+06  | 0.04436585E+02  |                 |         |         |         | 4 |
| SIH2CL    | 121986SI        | 1H              | 2CL             | 1               | G               | 0300.00 | 2000.00 | 1000.00 | 1 |
|           | 0.05555901E+02  | 0.04046479E-01  | -0.06581751E-05 | -0.05027548E-08 | 0.15991101E-12  |         |         |         | 2 |
|           | 0.01912428E+05  | -0.01906889E+02 | 0.01699256E+02  | 0.01961407E+00  | -0.02622973E-03 |         |         |         | 3 |
|           | 0.01936416E-06  | -0.05846399E-10 | 0.02743661E+05  | 0.01683132E+03  |                 |         |         |         | 4 |
| SIH2F     | 42489SI         | 1F              | 1H              | 2               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.06020398E+02  | 0.03074039E-01  | -0.03248886E-05 | -0.03052243E-08 | 0.07098090E-12  |         |         |         | 2 |
|           | -0.02347670E+06 | -0.05919595E+02 | 0.02782566E+02  | 0.09148257E-01  | -0.04186787E-05 |         |         |         | 3 |
|           | -0.05388971E-07 | 0.02412133E-10  | -0.02244201E+06 | 0.11528536E+02  |                 |         |         |         | 4 |
| SIH2F2    | 42489SI         | 1H              | 2F              | 2               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.07997762E+02  | 0.03911538E-01  | -0.04222679E-05 | -0.03913812E-08 | 0.09171569E-12  |         |         |         | 2 |
|           | -0.09682880E+06 | -0.16223999E+02 | 0.02701455E+02  | 0.14565451E-01  | -0.11633003E-05 |         |         |         | 3 |
|           | -0.09685830E-07 | 0.04769590E-10  | -0.09522440E+06 | 0.12006887E+02  |                 |         |         |         | 4 |
| SIH3      | 42489SI         | 1H              | 3               |                 | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.05015906E+02  | 0.03732750E-01  | -0.03609053E-05 | -0.03729193E-08 | 0.08468491E-12  |         |         |         | 2 |
|           | 0.02190233E+06  | -0.04291368E+02 | 0.02946733E+02  | 0.06466763E-01  | 0.05991653E-05  |         |         |         | 3 |
|           | -0.02218413E-07 | 0.03052669E-11  | 0.02270173E+06  | 0.07347948E+02  |                 |         |         |         | 4 |
| SIH3NH2   | 42489SI         | 1N              | 1H              | 5               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.08109945E+02  | 0.07215752E-01  | -0.06052251E-05 | -0.07086088E-08 | 0.15578638E-12  |         |         |         | 2 |
|           | -0.08999782E+05 | -0.16516504E+02 | 0.02936348E+02  | 0.16747041E-01  | -0.03232858E-05 |         |         |         | 3 |
|           | -0.09171970E-07 | 0.03979516E-10  | -0.07334716E+05 | 0.11414373E+02  |                 |         |         |         | 4 |
| SIH3NSIH3 | 42489SI         | 2N              | 1H              | 7               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.12652963E+02  | 0.10667481E-01  | -0.10073358E-05 | -0.10812221E-08 | 0.02452363E-11  |         |         |         | 2 |
|           | -0.12497210E+05 | -0.03441428E+03 | 0.02468749E+02  | 0.02940254E+00  | -0.06248179E-05 |         |         |         | 3 |
|           | -0.01731461E-06 | 0.07545261E-10  | -0.09209690E+05 | 0.02059559E+03  |                 |         |         |         | 4 |
| SIH3NSIH3 | 42489SI         | 2N              | 1H              | 6               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|           | 0.12014620E+02  | 0.09187517E-01  | -0.09159516E-05 | -0.09380967E-08 | 0.02156435E-11  |         |         |         | 2 |
|           | 0.01965065E+06  | -0.02978185E+03 | 0.02827574E+02  | 0.02580646E+00  | -0.04200477E-05 |         |         |         | 3 |
|           | -0.15038588E-07 | 0.06388324E-10  | 0.02265351E+06  | 0.01997012E+03  |                 |         |         |         | 4 |
| SIH4      | 121386SI        | 1H              | 4               |                 | G               | 0300.00 | 4000.00 | 1000.00 | 1 |
|           | 0.06893873E+02  | 0.04030500E-01  | -0.04183314E-05 | -0.02291394E-08 | 0.04384766E-12  |         |         |         | 2 |
|           | 0.11070374E+04  | -0.01749116E+03 | 0.02475166E+02  | 0.09003721E-01  | 0.02185394E-04  |         |         |         | 3 |
|           | -0.02681423E-07 | -0.06621080E-11 | 0.02925488E+05  | 0.07751014E+02  |                 |         |         |         | 4 |
| SIHCL2    | 121986SI        | 1H              | 1CL             | 2               | G               | 0300.00 | 2000.00 | 1000.00 | 1 |
|           | 0.07229734E+02  | 0.02869205E-01  | -0.08849876E-05 | -0.07495865E-09 | 0.05752338E-12  |         |         |         | 2 |
|           | -0.01971399E+06 | -0.07052663E+02 | 0.02368353E+02  | 0.02401088E+00  | -0.03717219E-03 |         |         |         | 3 |
|           | 0.02851997E-06  | -0.08530494E-10 | -0.01875884E+06 | 0.16145866E+02  |                 |         |         |         | 4 |

|       |                 |                 |                 |                 |                 |         |         |         |   |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|---------|---------|---|
| SIHF  | 42489SI         | 1F              | 1H              | 1               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|       | 0.05073508E+02  | 0.15332789E-02  | -0.01840658E-05 | -0.14400376E-09 | 0.03452517E-12  |         |         |         | 2 |
|       | -0.01973879E+06 | -0.10795069E+01 | 0.03223727E+02  | 0.04981220E-01  | -0.03173051E-05 |         |         |         | 3 |
|       | -0.02822231E-07 | 0.12478316E-11  | -0.01914167E+06 | 0.08906423E+02  |                 |         |         |         | 4 |
| SIHF2 | 42489SI         | 1H              | 1F              | 2               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|       | 0.07216536E+02  | 0.02253240E-01  | -0.02737472E-05 | -0.02173460E-08 | 0.05255331E-12  |         |         |         | 2 |
|       | -0.07280241E+06 | -0.09783487E+02 | 0.03377237E+02  | 0.10366072E-01  | -0.12390823E-05 |         |         |         | 3 |
|       | -0.07267981E-07 | 0.03794989E-10  | -0.07168358E+06 | 0.10521894E+02  |                 |         |         |         | 4 |
| SIHF3 | 42489SI         | 1H              | 1F              | 3               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|       | 0.09363567E+02  | 0.02947555E-01  | -0.03577633E-05 | -0.02858224E-08 | 0.06915728E-12  |         |         |         | 2 |
|       | -0.14860736E+06 | -0.02169452E+03 | 0.03918053E+02  | 0.14639172E-01  | -0.01856069E-04 |         |         |         | 3 |
|       | -0.10582003E-07 | 0.05617543E-10  | -0.14704386E+06 | 0.07024261E+02  |                 |         |         |         | 4 |
| SIN   | 42489SI         | 1N              | 1               | G               | 0300.00         | 3000.00 | 1000.00 | 1       |   |
|       | 0.04122909E+02  | 0.03521457E-02  | -0.07161080E-06 | -0.02154956E-09 | 0.06667570E-13  |         |         |         | 2 |
|       | 0.05683927E+06  | 0.02389837E+02  | 0.03149181E+02  | 0.02584376E-01  | -0.05804624E-05 |         |         |         | 3 |
|       | -0.01805626E-07 | 0.10410949E-11  | 0.05710563E+06  | 0.07474389E+02  |                 |         |         |         | 4 |
| SINH  | 42489SI         | 1N              | 1H              | 1               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|       | 0.04928800E+02  | 0.16286244E-02  | -0.13671971E-06 | -0.13904604E-09 | 0.02998968E-12  |         |         |         | 2 |
|       | 0.01767789E+06  | -0.02823472E+02 | 0.03166974E+02  | 0.05805822E-01  | -0.09524443E-05 |         |         |         | 3 |
|       | -0.03991892E-07 | 0.02283188E-10  | 0.01813560E+06  | 0.06298439E+02  |                 |         |         |         | 4 |
| SINH2 | 42489SI         | 1N              | 1H              | 2               | G               | 0300.00 | 3000.00 | 1000.00 | 1 |
|       | 0.05186435E+02  | 0.03016656E-01  | -0.02165476E-05 | -0.02722658E-08 | 0.05706182E-12  |         |         |         | 2 |
|       | 0.02270507E+06  | -0.12421399E+01 | 0.03362769E+02  | 0.07261175E-01  | -0.08721233E-05 |         |         |         | 3 |
|       | -0.04400014E-07 | 0.02419532E-10  | 0.02318445E+06  | 0.08223867E+02  |                 |         |         |         | 4 |
| SN    | 121286S         | 1N              | 1               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.03888286E+02  | 0.06778427E-02  | -0.02725308E-05 | 0.05135927E-09  | -0.03593836E-13 |         |         |         | 2 |
|       | 0.03044496E+06  | 0.04194291E+02  | 0.03407345E+02  | 0.01797887E-01  | -0.02018969E-04 |         |         |         | 3 |
|       | 0.02107857E-07  | -0.09527593E-11 | 0.03062373E+06  | 0.06821481E+02  |                 |         |         |         | 4 |
| S0    | 121286S         | 10              | 1               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.04021077E+02  | 0.02584856E-02  | 0.08948142E-06  | -0.03580144E-09 | 0.03228430E-13  |         |         |         | 2 |
|       | -0.07119620E+04 | 0.03452522E+02  | 0.03080401E+02  | 0.01803105E-01  | 0.06705022E-05  |         |         |         | 3 |
|       | -0.02069005E-07 | 0.08514657E-11  | -0.03986163E+04 | 0.08581028E+02  |                 |         |         |         | 4 |
| S02   | 121286S         | 10              | 2               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.05254498E+02  | 0.01978545E-01  | -0.08204226E-05 | 0.15763830E-09  | -0.11204512E-13 |         |         |         | 2 |
|       | -0.03756885E+06 | -0.11460563E+01 | 0.02911438E+02  | 0.08103022E-01  | -0.06906710E-04 |         |         |         | 3 |
|       | 0.03329015E-07  | -0.08777121E-11 | -0.03687881E+06 | 0.11117403E+02  |                 |         |         |         | 4 |
| S03   | 121286S         | 10              | 3               | G               | 0300.00         | 5000.00 | 1000.00 | 1       |   |
|       | 0.07050668E+02  | 0.03246560E-01  | -0.14088974E-05 | 0.02721535E-08  | -0.01942364E-12 |         |         |         | 2 |
|       | -0.05020667E+06 | -0.11064426E+02 | 0.02575282E+02  | 0.15150916E-01  | -0.12298717E-04 |         |         |         | 3 |
|       | 0.04240257E-07  | -0.05266812E-11 | -0.04894410E+06 | 0.12195116E+02  |                 |         |         |         | 4 |

# APPENDIX C. GRAPHICAL REPRESENTATION OF DATA BASE

Species: AL

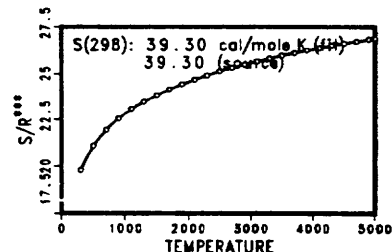
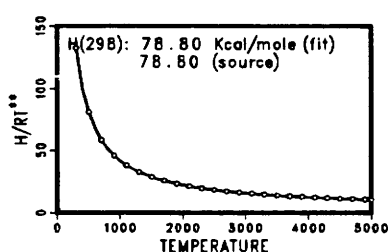
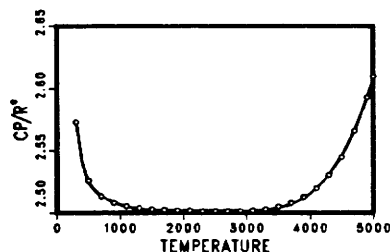
ALUMINUM, MONATOMIC

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-0600K   | 0.02736825E+02 | -0.05912374E-02 | -0.04033937E-05 | 0.02322343E-07  | -0.01705599E-10 | 0.03886794E+06 | 0.04363879E+02 |
| 0600-5000K   | 0.02559589E+02 | -0.10632239E-03 | 0.07202828E-06  | -0.02121105E-09 | 0.02289429E-13  | 0.03890214E+06 | 0.05234522E+02 |



Source: SNL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

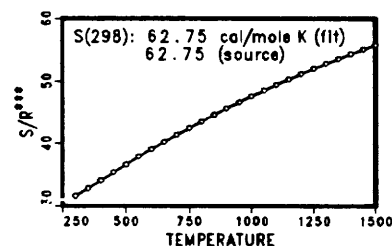
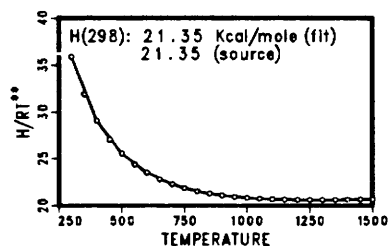
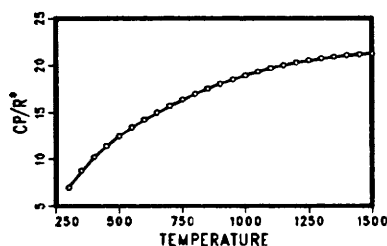
Species: AL2H6

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|-----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | -0.06800681E+02 | 0.05080744E+00 | 0.10397471E-04 | -0.11195819E-06 | 0.08459155E-09 | 0.10605371E+05 | 0.05554526E+03 |
| 0600-1500K   | 0.02634884E+02  | 0.02135952E+00 | 0.03154151E-05 | -0.07684674E-07 | 0.02335831E-10 | 0.08871346E+05 | 0.09827515E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: AL2ME6

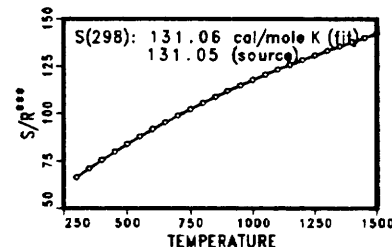
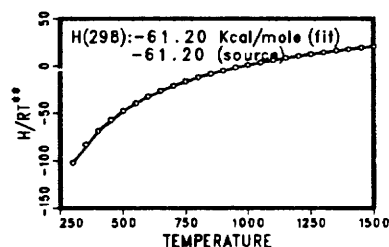
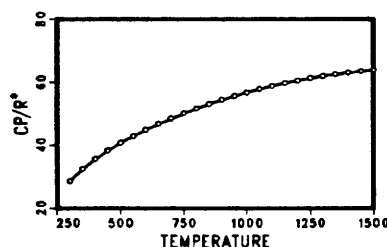
("ME" = CH<sub>3</sub>, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.07159750E+01 | 0.10671087E+00 | 0.02117604E-03 | -0.02193211E-05 | 0.16441438E-09 | -0.03515546E+06 | 0.03890762E+03  |
| 0600-1500K   | 0.01773147E+03  | 0.04935747E+00 | 0.11968535E-05 | -0.16398263E-07 | 0.04890867E-10 | -0.03855560E+06 | -0.05053298E+03 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

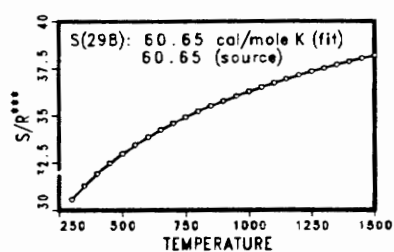
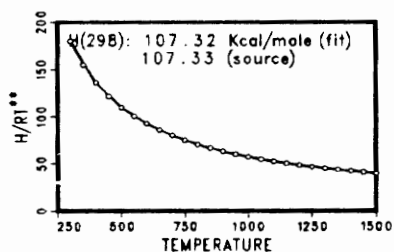
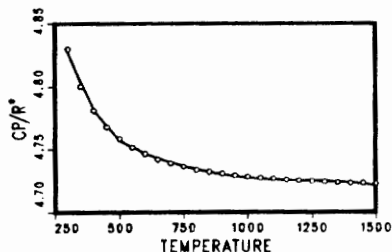
Species: ALAS

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-0600K   | 0.05047764E+02 | -0.06419947E-02 | -0.14320714E-05 | 0.04754390E-07 | -0.03297621E-10 | 0.05254264E+06 | 0.01985205E+02 |
| 0600-1500K   | 0.04790026E+02 | -0.01908225E-03 | -0.01983390E-05 | 0.02239358E-08 | -0.06904706E-12 | 0.05259290E+06 | 0.03259703E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ALH

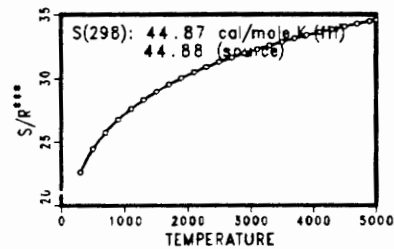
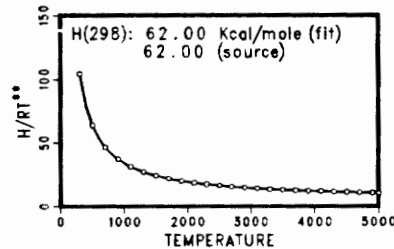
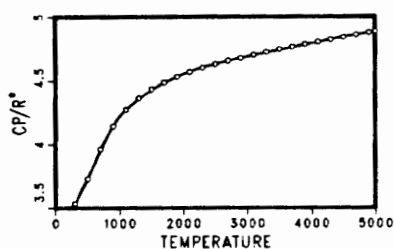
ALUMINUM MONOHYDRIDE

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03071503E+02 | 0.02165549E-01 | -0.03275638E-04 | 0.04136983E-07 | -0.01877120E-10 | 0.03021221E+06 | 0.04548855E+02 |
| 1000-5000K   | 0.03392644E+02 | 0.12153990E-02 | -0.04676595E-05 | 0.08691624E-09 | -0.06022668E-13 | 0.03006845E+06 | 0.02758899E+02 |



Source: SNL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

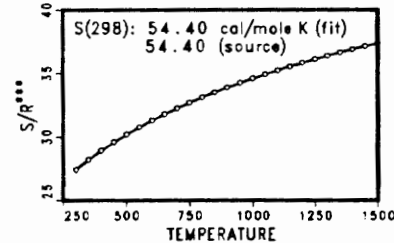
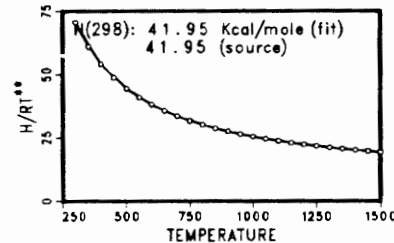
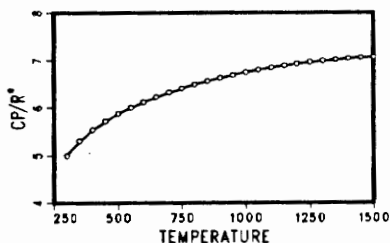
Species: ALH2

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.02442136E+02 | 0.09915913E-01 | 0.02471082E-05  | -0.02119583E-06 | 0.01710233E-09 | 0.01997567E+06 | 0.10652699E+02 |
| 0600-1500K   | 0.04486543E+02 | 0.03128831E-01 | -0.01969438E-05 | -0.01060304E-08 | 0.03497468E-11 | 0.01960959E+06 | 0.08167897E+01 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

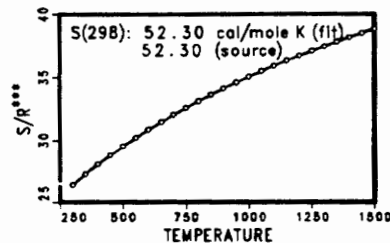
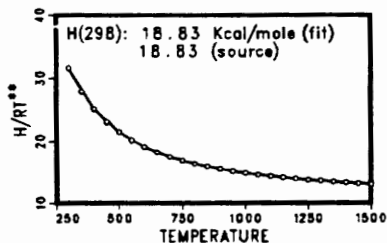
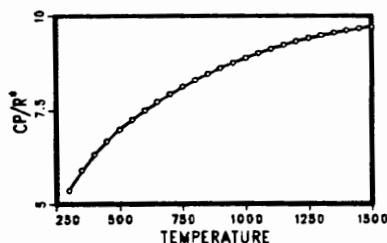
Species: ALH3

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.10083231E+01 | 0.16403245E-01 | 0.01976746E-04  | -0.03528558E-06 | 0.02753377E-09 | 0.08484656E+05 | 0.15858377E+02 |
| 0600-1500K   | 0.04186837E+02 | 0.06159249E-01 | -0.03877593E-06 | -0.02061928E-07 | 0.06600276E-11 | 0.07908078E+05 | 0.05134396E+01 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: ALME

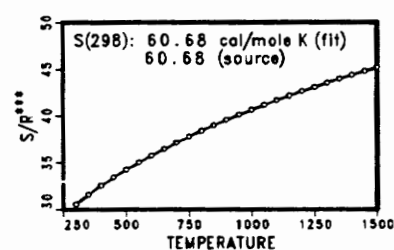
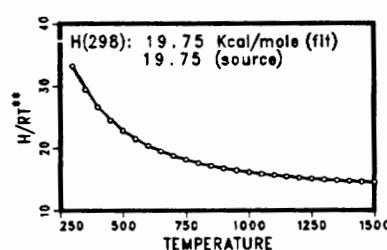
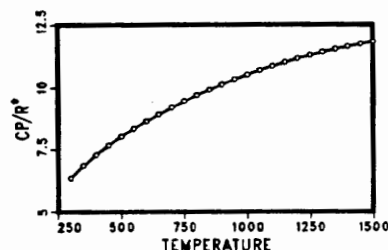
("ME" = CH<sub>3</sub>, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.02664176E+02 | 0.13249141E-01 | 0.02525847E-04 | -0.02394396E-06 | 0.01761854E-09 | 0.08574173E+05 | 0.11474494E+02 |
| 0600-1500K   | 0.04662737E+02 | 0.07097939E-01 | 0.02520013E-05 | -0.02114863E-07 | 0.06097489E-11 | 0.08203227E+05 | 0.01769244E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: ALME2

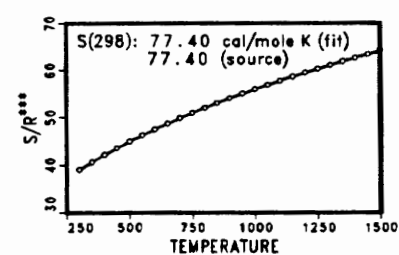
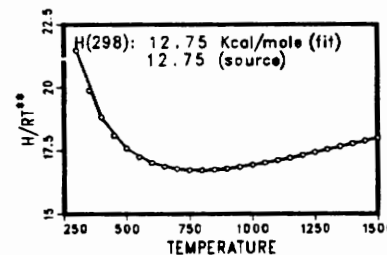
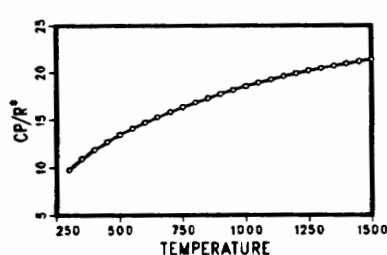
("ME" = CH<sub>3</sub>, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.09494573E+01 | 0.03206353E+00 | 0.06134020E-04 | -0.06500042E-06 | 0.04911485E-09 | 0.04761408E+05 | 0.02419465E+03  |
| 0600-1500K   | 0.06481282E+02 | 0.14746049E-01 | 0.05816529E-05 | -0.04621347E-07 | 0.13960405E-11 | 0.03745072E+05 | -0.02603325E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: ALME3

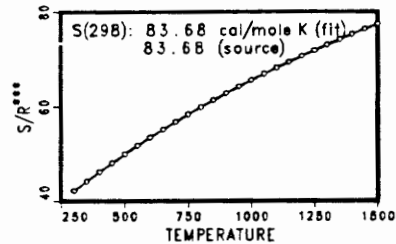
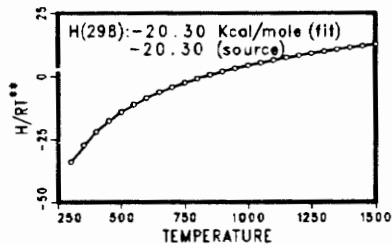
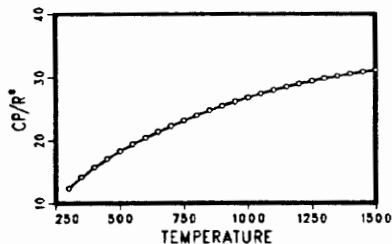
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.07027567E+01 | 0.04682764E+00 | 0.11499028E-04 | -0.09160441E-06 | 0.06687293E-09 | -0.12037989E+05 | 0.03232771E+03  |
| 0600-1500K   | 0.06654948E+02  | 0.02455144E+00 | 0.11765745E-05 | -0.07815023E-07 | 0.02255622E-10 | -0.13409524E+05 | -0.03454481E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: AR

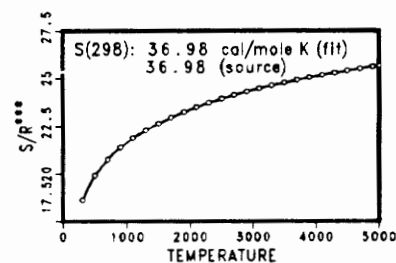
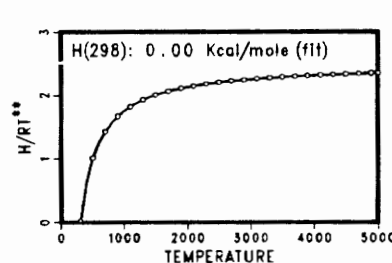
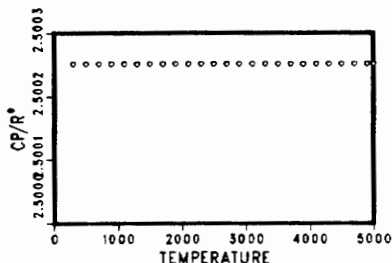
ARGON, MONATOMIC (REF ST)

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|----------------|----------------|-----------------|----------------|
| 0300-1000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | -0.07453750E+04 | 0.04366000E+02 |
| 1000-5000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | -0.07453750E+04 | 0.04366000E+02 |



Source: NASA FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: AR+

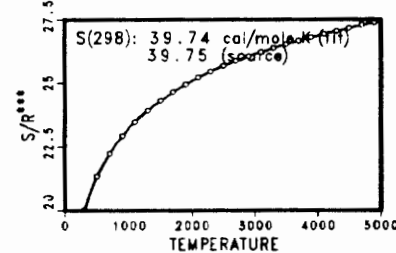
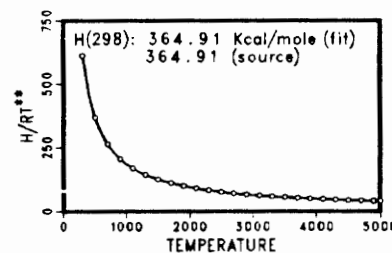
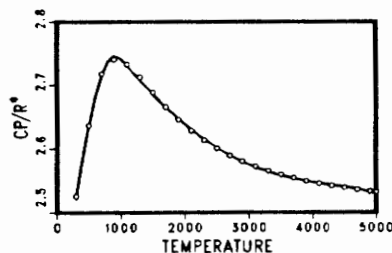
ARGON, UNIPOSITIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02301341E+02 | 0.08035528E-02  | -0.01758805E-05 | -0.01781093E-08 | -0.08937268E-13 | 0.01829281E+07 | 0.06659358E+02 |
| 1000-5000K   | 0.02864864E+02 | -0.12035732E-03 | -0.10651992E-07 | 0.09074839E-10  | -0.09623876E-14 | 0.01827230E+07 | 0.03543584E+02 |



Source: SNL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

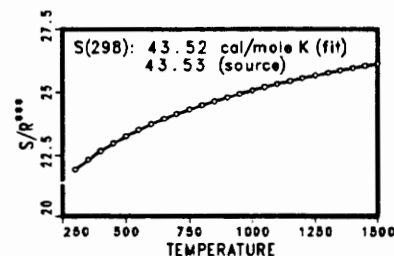
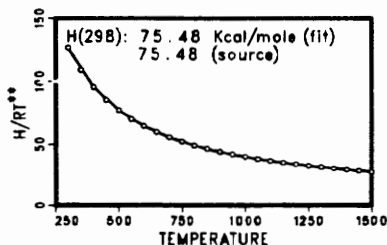
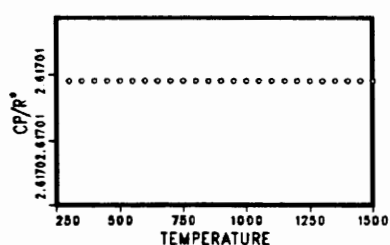
Species: AS

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.02617010E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.03720454E+06 | 0.06995524E+02 |
| 0600-1500K   | 0.02617010E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.03720454E+06 | 0.06995524E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

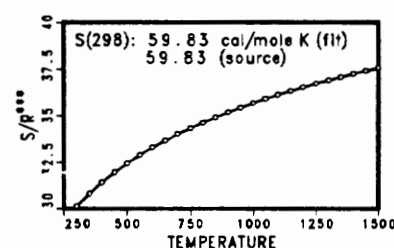
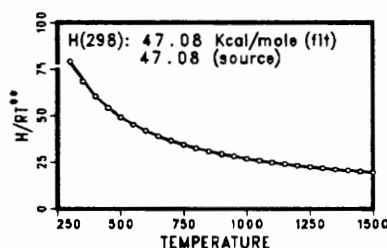
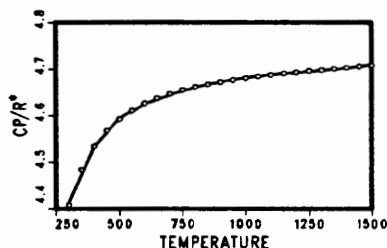
Species: AS2

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.03682891E+02 | 0.03121811E-01 | -0.10740519E-05 | -0.05629472E-07 | 0.05178811E-10 | 0.02247355E+06 | 0.08283423E+02 |
| 0600-1500K   | 0.04394201E+02 | 0.05389968E-02 | -0.02379401E-05 | -0.06541924E-09 | 0.05184186E-12 | 0.02235093E+06 | 0.04897918E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

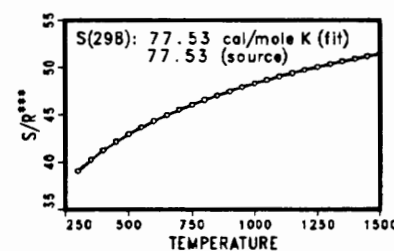
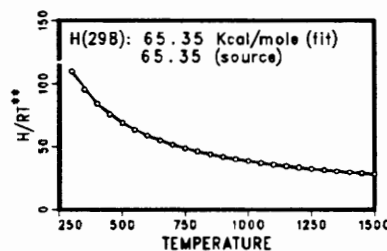
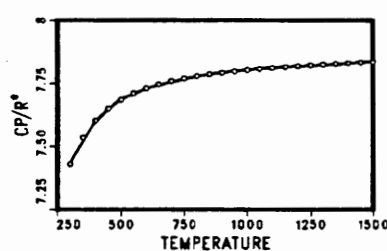
Species: AS3

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.06403142E+02 | 0.04477098E-01 | -0.01866642E-04 | -0.07394750E-07 | 0.07012752E-10 | 0.03080965E+06 | 0.13371355E+01  |
| 0600-1500K   | 0.07404036E+02 | 0.07818425E-02 | -0.03918297E-05 | -0.05203629E-09 | 0.06291907E-12 | 0.03063825E+06 | -0.03417323E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



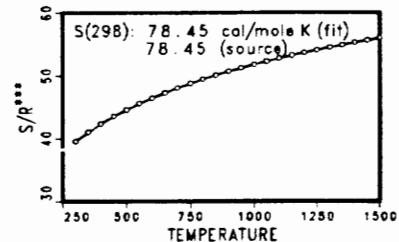
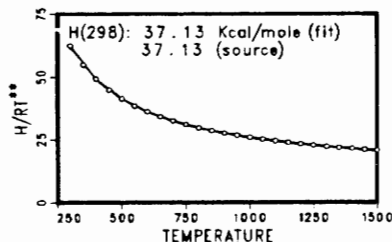
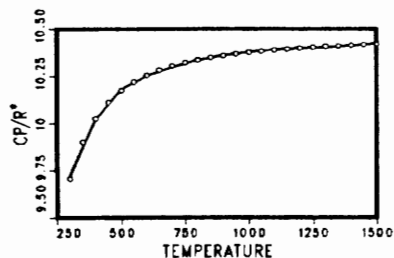
Species: AS4

GAS

As of: 6/29/87

Fit  
Coefficients

|            | $a_1$          | $a_2$          | $a_3$           | $a_4$           | $a_5$          | $a_6$          | $a_7$           |
|------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K | 0.07853760E+02 | 0.07916509E-01 | -0.02329820E-04 | -0.15263119E-07 | 0.13774348E-10 | 0.16036290E+05 | -0.07409755E+02 |
| 0600-1500K | 0.09695766E+02 | 0.13062585E-02 | -0.05519564E-05 | -0.02150873E-08 | 0.14579349E-12 | 0.15717321E+05 | -0.16188696E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASALME

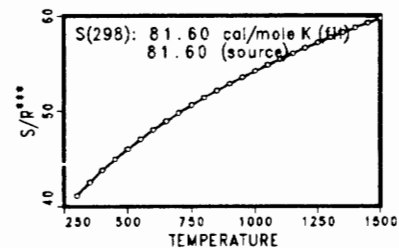
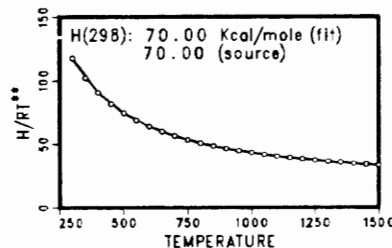
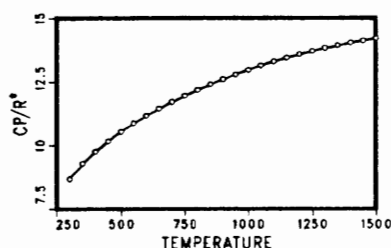
("ME" = CH<sub>3</sub>, METHYL)

GAS

As of: 6/29/87

Fit  
Coefficients

|            | $a_1$          | $a_2$          | $a_3$          | $a_4$           | $a_5$          | $a_6$          | $a_7$           |
|------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K | 0.04053423E+02 | 0.01726125E+00 | 0.01833498E-04 | -0.03386952E-06 | 0.02626980E-09 | 0.03329309E+06 | 0.12996653E+02  |
| 0600-1500K | 0.07127107E+02 | 0.07357863E-01 | 0.02300796E-06 | -0.02226398E-07 | 0.06927227E-11 | 0.03273438E+06 | -0.01847179E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASALME2

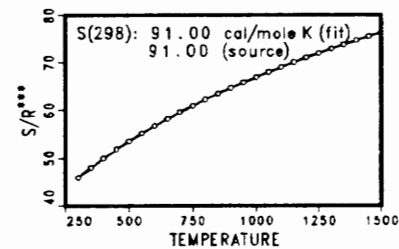
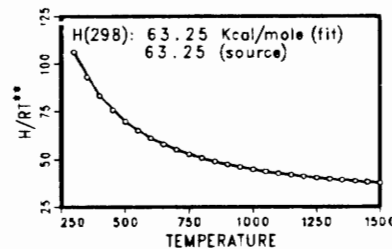
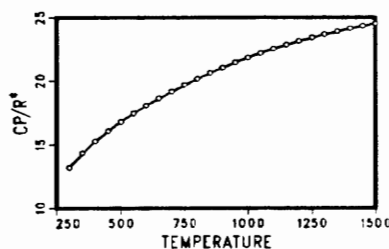
("ME" = CH<sub>3</sub>, METHYL)

GAS

As of: 6/29/87

Fit  
Coefficients

|            | $a_1$          | $a_2$          | $a_3$          | $a_4$           | $a_5$          | $a_6$          | $a_7$           |
|------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K | 0.04808530E+02 | 0.03067687E+00 | 0.05048000E-04 | -0.05908099E-06 | 0.04462290E-09 | 0.02908816E+06 | 0.09471621E+02  |
| 0600-1500K | 0.09909938E+02 | 0.14638499E-01 | 0.04118730E-05 | -0.04444657E-07 | 0.13295010E-11 | 0.02815111E+06 | -0.15235312E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASGAET

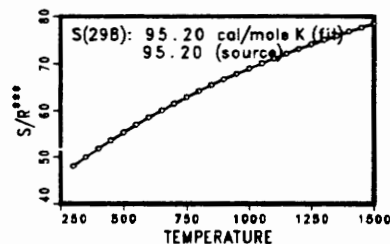
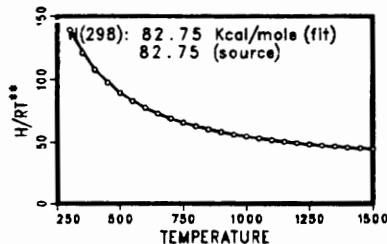
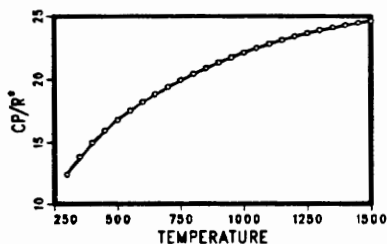
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.06364698E+01 | 0.04382467E+00 | 0.06144686E-04 | -0.09491641E-06 | 0.07374197E-09 | 0.03960893E+06 | 0.03164673E+03  |
| 0600-1500K   | 0.09081073E+02 | 0.16746316E-01 | 0.12831301E-06 | -0.05590435E-07 | 0.01781314E-10 | 0.03807443E+06 | -0.09142782E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASGAET2

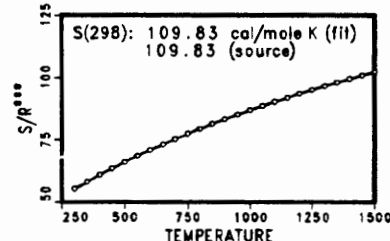
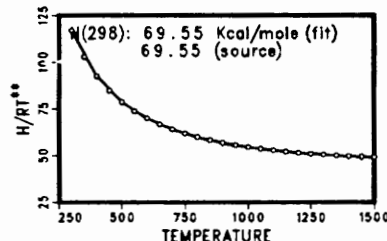
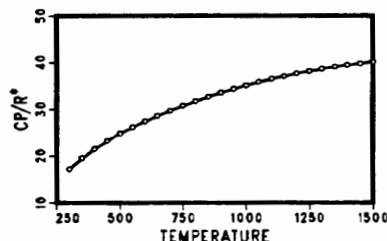
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | -0.03539248E+01 | 0.06369772E+00 | 0.13597417E-04 | -0.12861423E-06 | 0.09572181E-09 | 0.03236903E+06 | 0.03865086E+03  |
| 0600-1500K   | 0.10324288E+02  | 0.03073570E+00 | 0.10863354E-05 | -0.09971948E-07 | 0.02945979E-10 | 0.03039490E+06 | -0.13164016E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASGAME

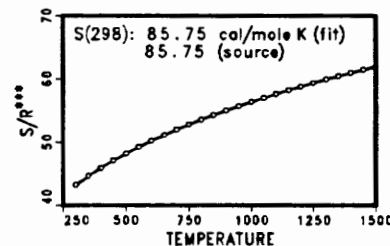
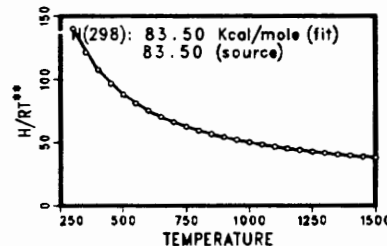
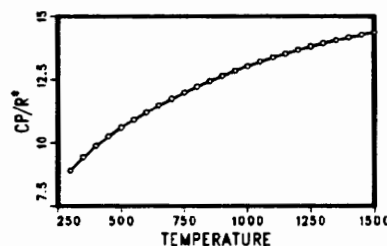
("ME" = CH3, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.04877266E+02 | 0.14825589E-01 | 0.16521240E-05 | -0.02712058E-06 | 0.02080195E-09 | 0.03994071E+06 | 0.11076703E+02  |
| 0600-1500K   | 0.07322183E+02 | 0.06995478E-01 | 0.10693509E-06 | -0.01995283E-07 | 0.06040446E-11 | 0.03949448E+06 | -0.07416680E+01 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASGAME2

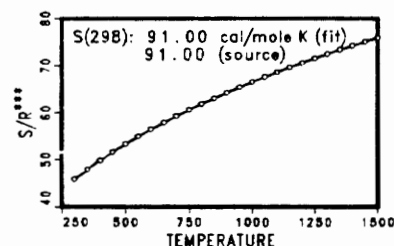
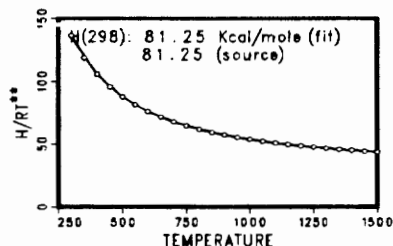
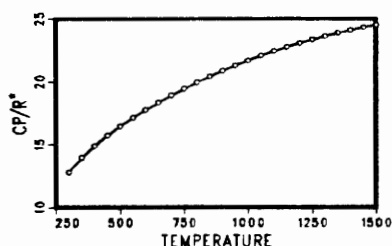
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.04382076E+02 | 0.03056344E+00 | 0.05477067E-04 | -0.05834108E-06 | 0.04373509E-09 | 0.03827434E+06 | 0.11911109E+02  |
| 0600-1500K   | 0.09352436E+02 | 0.15048197E-01 | 0.05157975E-05 | -0.04553518E-07 | 0.13487630E-11 | 0.03735855E+06 | -0.12181144E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: ASGAMEH

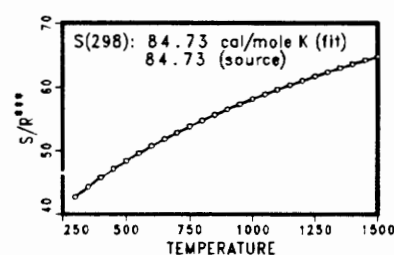
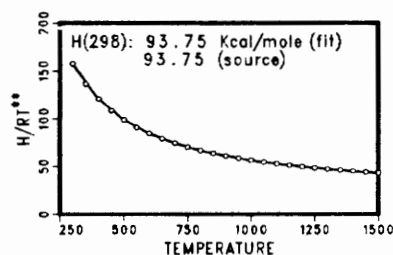
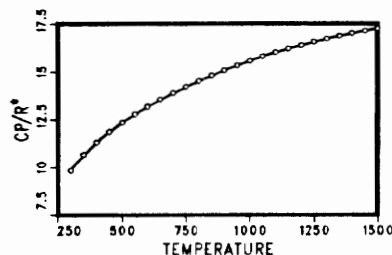
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.03585119E+02 | 0.02336317E+00 | 0.02873356E-04 | -0.04737894E-06 | 0.03674461E-09 | 0.04512702E+06 | 0.15471604E+02  |
| 0600-1500K   | 0.07842794E+02 | 0.09682097E-01 | 0.10603061E-06 | -0.02991402E-07 | 0.09382673E-11 | 0.04435297E+06 | -0.05093455E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

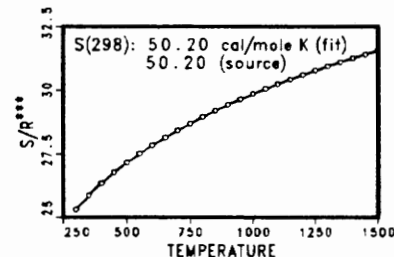
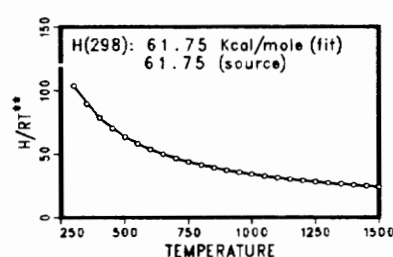
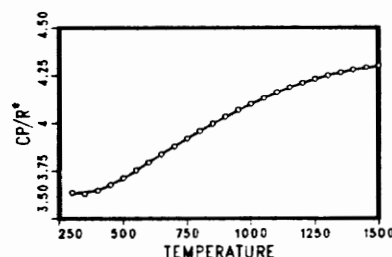
Species: ASH

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-0600K   | 0.03865843E+02 | -0.11575710E-02 | -0.03494371E-05 | 0.07079686E-07  | -0.06014027E-10 | 0.02996829E+06 | 0.03549869E+02 |
| 0600-1500K   | 0.03219848E+02 | 0.10012498E-02  | -0.04674997E-08 | -0.11076533E-09 | -0.09254321E-13 | 0.03008175E+06 | 0.06647311E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

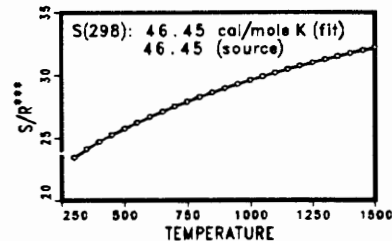
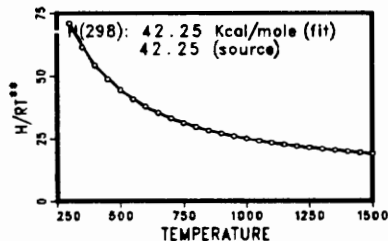
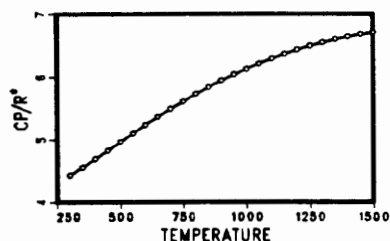
Species: ASH2

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|-----------------|----------------|----------------|
| 0300-0600K   | 0.03778945E+02 | 0.01759233E-01 | 0.08070806E-05 | 0.02358763E-07  | -0.03043521E-10 | 0.02004661E+06 | 0.12729740E+01 |
| 0600-1500K   | 0.03428307E+02 | 0.03181140E-01 | 0.14604843E-06 | -0.07937145E-08 | 0.01694413E-11  | 0.02010282E+06 | 0.02904703E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet\bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet\bullet\bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

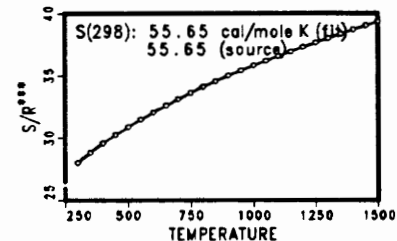
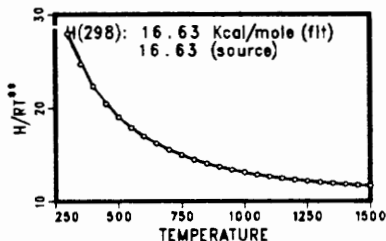
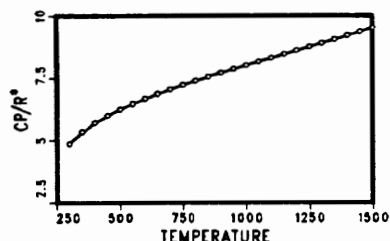
Species: ASH3

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.09446356E+01 | 0.15084686E-01 | 0.12016960E-05 | -0.03397465E-06 | 0.02767656E-09 | 0.07459168E+05 | 0.01832267E+03 |
| 0600-1500K   | 0.04172022E+02 | 0.04371322E-01 | 0.02177574E-05 | -0.11832641E-08 | 0.04536373E-11 | 0.06882915E+05 | 0.02803476E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet\bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet\bullet\bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASME

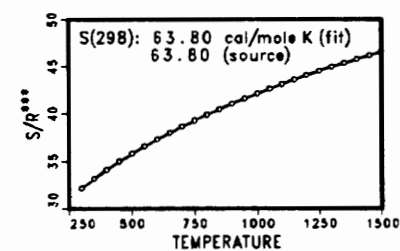
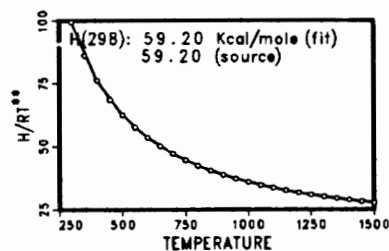
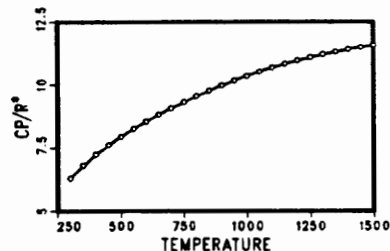
("ME" = CH<sub>3</sub>, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.02625270E+02 | 0.13252423E-01 | 0.02441628E-04 | -0.02419566E-06 | 0.01786943E-09 | 0.02844080E+06 | 0.13273359E+02 |
| 0600-1500K   | 0.04657260E+02 | 0.06976297E-01 | 0.02147556E-05 | -0.02101159E-07 | 0.06082149E-11 | 0.02806422E+06 | 0.03409834E+02 |



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet\bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet\bullet\bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASME2

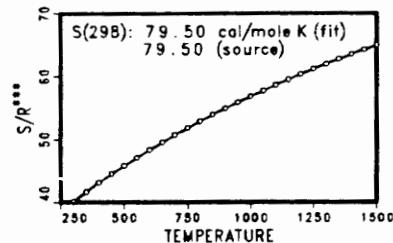
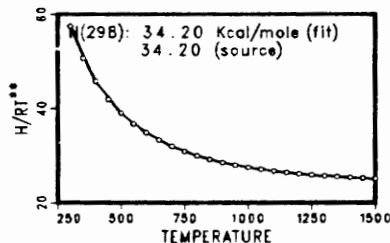
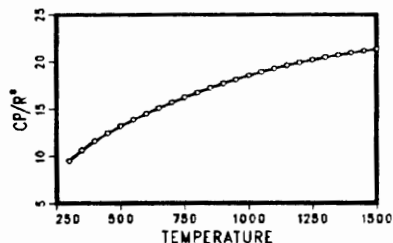
("ME" = CH3,METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.13903998E+01 | 0.02923331E+00 | 0.06598870E-04 | -0.05620559E-06 | 0.04130367E-09 | 0.15533022E+05 | 0.02349980E+03 |
| 0600-1500K   | 0.05981395E+02 | 0.15212837E-01 | 0.06993355E-05 | -0.04721619E-07 | 0.13699115E-11 | 0.14679847E+05 | 0.11927411E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: ASME3

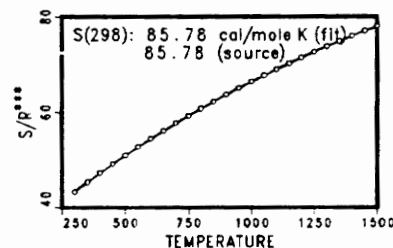
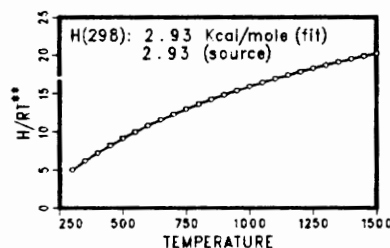
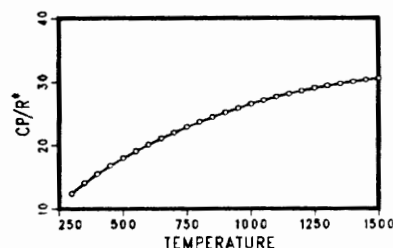
("ME" = CH3,METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | 0.02667388E+01 | 0.04253171E+00 | 0.11651064E-04 | -0.07914706E-06 | 0.05603126E-09 | -0.04685539E+04 | 0.02904590E+03  |
| 0600-1500K   | 0.06347764E+02 | 0.02466454E+00 | 0.11546286E-05 | -0.07877435E-07 | 0.02202225E-10 | -0.16173225E+04 | -0.06316786E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C

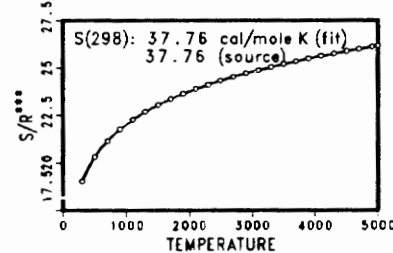
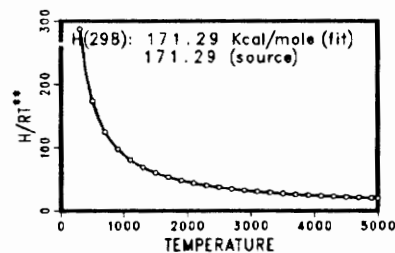
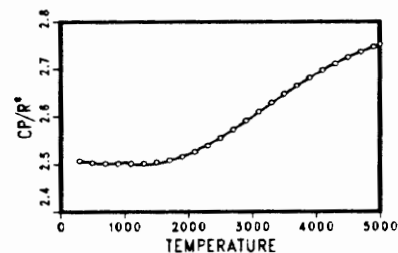
CARBON, MONATOMIC

GAS

As of: 12/10/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02498584E+02 | 0.08085776E-03  | -0.02697697E-05 | 0.03040729E-08  | -0.11066518E-12 | 0.08545878E+06 | 0.04753459E+02 |
| 1000-5000K   | 0.02602087E+02 | -0.01787081E-02 | 0.09087041E-06  | -0.11499333E-10 | 0.03310844E-14  | 0.08542154E+06 | 0.04195177E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C(S)

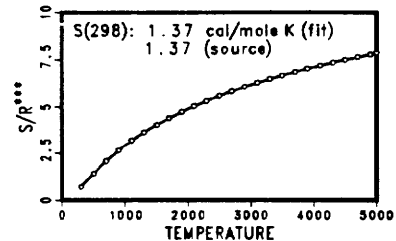
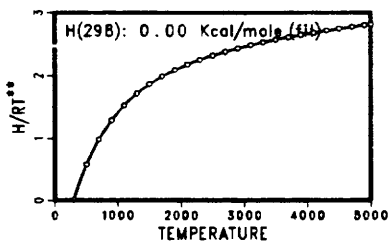
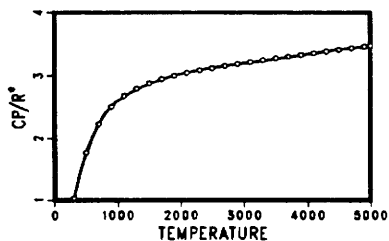
CARBON (REF ST), GRAPHITE

SOLID

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | -0.06705661E+01 | 0.07181499E-01 | -0.05632921E-04 | 0.02142298E-07 | -0.04168562E-11 | -0.07339498E+03 | 0.02601595E+02  |
| 1000-5000K   | 0.14901664E+01  | 0.16621256E-02 | -0.06687204E-05 | 0.12908796E-09 | -0.09205334E-13 | -0.07074018E+04 | -0.08717785E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C+

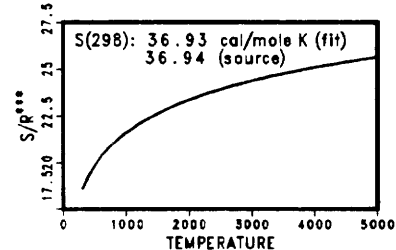
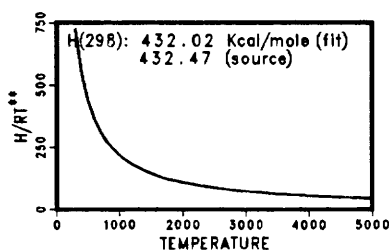
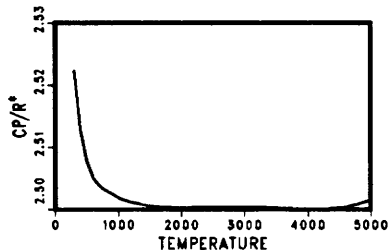
CARBON, UNIPOSITIVE ION

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.02595384E+02 | -0.04068664E-02 | 0.06892366E-05 | -0.05266488E-08 | 0.15083378E-12 | 0.02166628E+07 | 0.03895729E+02 |
| 1000-5000K   | 0.02511827E+02 | -0.01735978E-03 | 0.09504267E-07 | -0.02218851E-10 | 0.01862189E-14 | 0.02166772E+07 | 0.04286130E+02 |



Source: NASA FIT TO NASA LEWIS DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C-

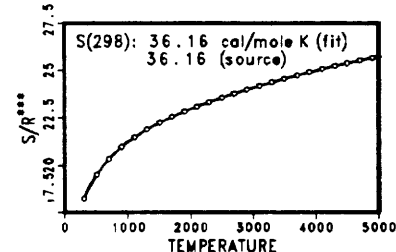
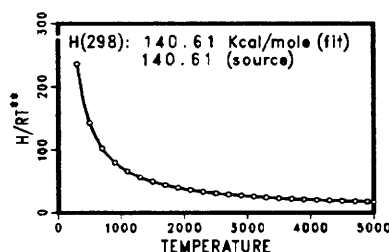
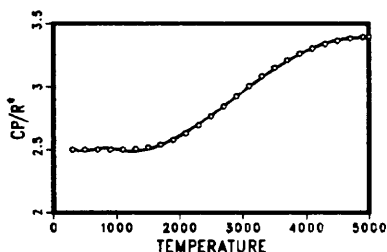
CARBON, UNINEGATIVE ION

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.02783902E+02 | -0.01774287E-01 | 0.03696760E-04 | -0.03066693E-07 | 0.08637622E-11 | 0.06998511E+06 | 0.02726281E+02 |
| 1000-5000K   | 0.02990221E+02 | -0.09184596E-02 | 0.05055560E-05 | -0.07703410E-09 | 0.03163271E-13 | 0.06983931E+06 | 0.12594533E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2

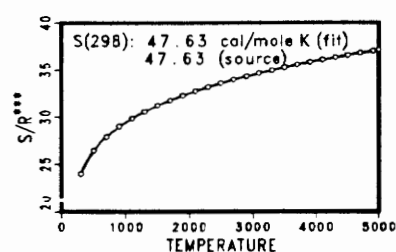
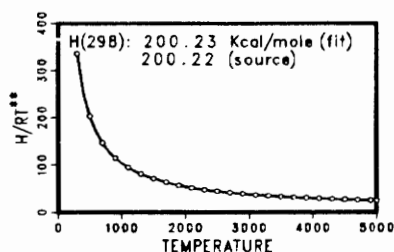
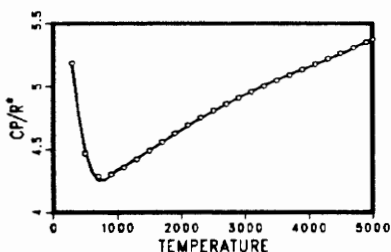
CARBON, DIATOMIC

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.06996045E+02 | -0.07400601E-01 | 0.03234703E-04 | 0.04802535E-07  | -0.03295917E-10 | 0.09897487E+06 | -0.13862268E+02 |
| 1000-5000K   | 0.04135978E+02 | 0.06531618E-03  | 0.01837099E-05 | -0.05295085E-09 | 0.04712137E-13  | 0.09967272E+06 | 0.07472923E+01  |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2-

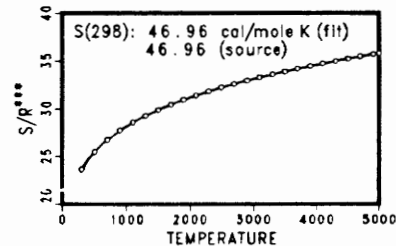
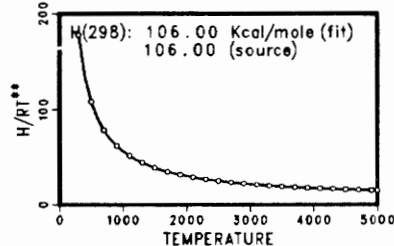
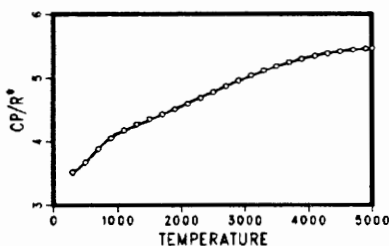
DIMERIC CARBON, UNINEGATIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03468011E+02 | -0.02352874E-02 | 0.12439123E-05 | 0.04705960E-08  | -0.08164274E-11 | 0.05231215E+06 | 0.03886699E+02 |
| 1000-5000K   | 0.03796891E+02 | 0.02530049E-02  | 0.09709118E-06 | -0.16148038E-10 | -0.03212893E-15 | 0.05207981E+06 | 0.16581468E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2F6

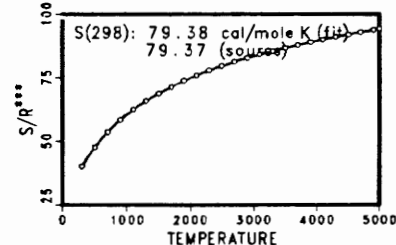
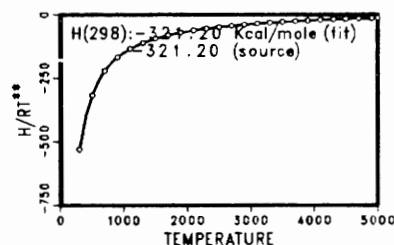
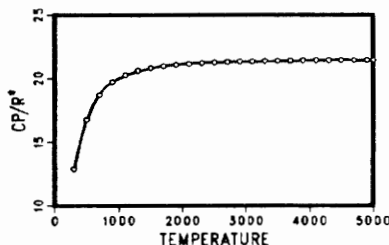
HEXAFLUOROETHANE

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.03577448E+02 | 0.03913670E+00 | -0.02714862E-03 | 0.04348459E-08 | 0.04007135E-10  | -0.16421741E+06 | 0.09098384E+02  |
| 1000-5000K   | 0.16020573E+02 | 0.06273007E-01 | -0.02797778E-04 | 0.05517547E-08 | -0.04004651E-12 | -0.16756543E+06 | -0.05519459E+03 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2H

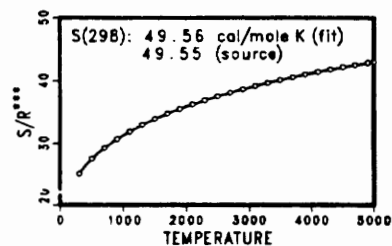
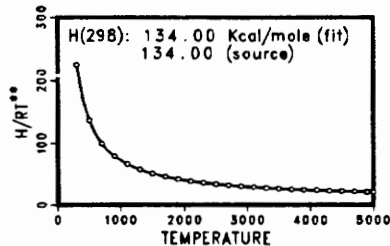
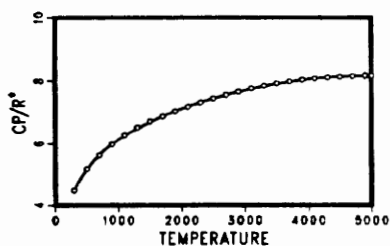
CCH RADICAL

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03050667E+02 | 0.06051674E-01 | -0.04956634E-04 | 0.02804159E-07 | -0.08193332E-11 | 0.06630011E+06 | 0.05954361E+02  |
| 1000-5000K   | 0.04427688E+02 | 0.02216268E-01 | -0.06048952E-05 | 0.09882517E-09 | -0.07351179E-13 | 0.06590415E+06 | -0.11994418E+01 |



Source: SNLL FIT TO JANAF TABLES WITH H298=134 PER MILLER

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2H2

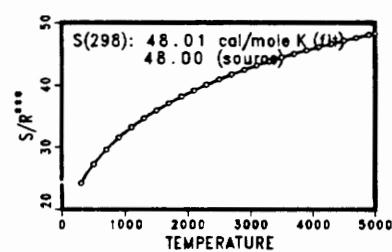
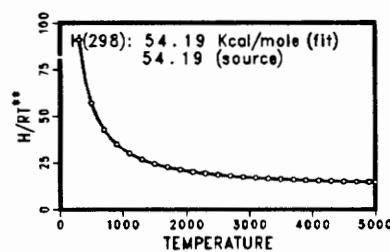
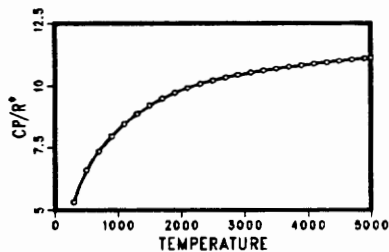
ACETYLENE

GAS

As of: 12/13/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02013562E+02 | 0.15190446E-01 | -0.16163189E-04 | 0.09078992E-07 | -0.01912746E-10 | 0.02612444E+06 | 0.08805378E+02  |
| 1000-5000K   | 0.04436770E+02 | 0.05376039E-01 | -0.01912816E-04 | 0.03286379E-08 | -0.02156709E-12 | 0.02566766E+06 | -0.02800338E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2H3

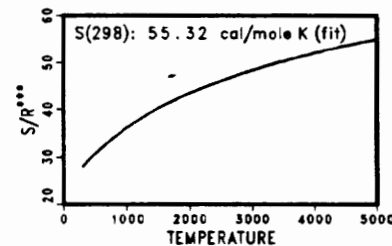
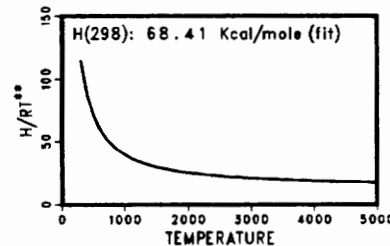
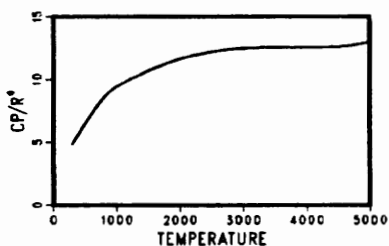
VINYL-RAD

GAS

As of: 1/27/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02459276E+02 | 0.07371476E-01 | 0.02109872E-04  | -0.13216421E-08 | -0.11847838E-11 | 0.03335225E+06 | 0.11556202E+02  |
| 1000-5000K   | 0.05933468E+02 | 0.04017745E-01 | -0.03966739E-05 | -0.14412666E-09 | 0.02378643E-12  | 0.03185434E+06 | -0.08530313E+02 |



Source: RECALC. OF BURCAT FIT (TECHNION), H298=68.4 PER MILLER

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



Species: C2H4

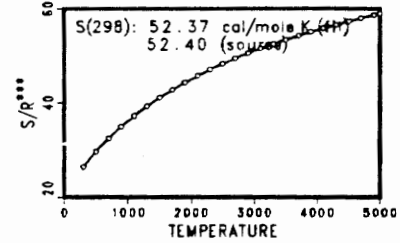
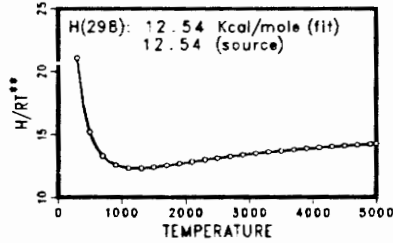
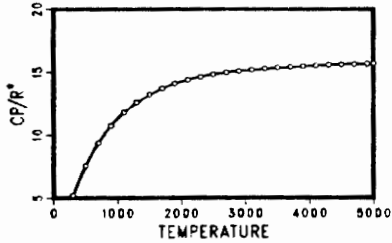
ETHYLENE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|-----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | -0.08514880E+01 | 0.02796162E+00 | -0.03388677E-03 | 0.02785152E-06 | -0.09737879E-10 | 0.05573046E+05 | 0.02421148E+03 |
| 1000-5000K   | 0.03528418E+02  | 0.11485185E-01 | -0.04418385E-04 | 0.07844600E-08 | -0.05266848E-12 | 0.04428288E+05 | 0.02230389E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2H5

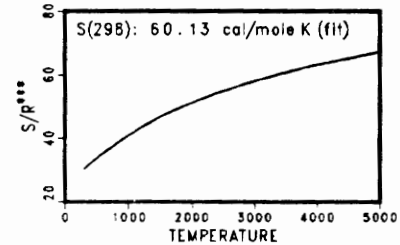
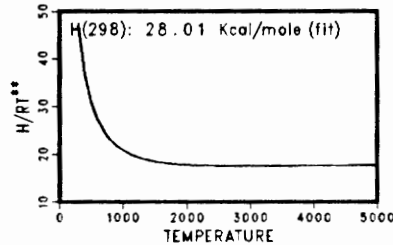
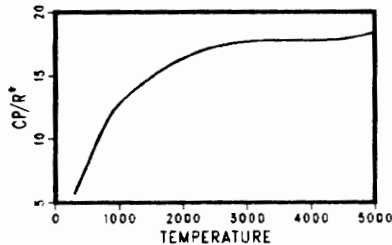
ETHYL RAD

GAS

As of: 1/23/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02690701E+02 | 0.08719133E-01 | 0.04419838E-04  | 0.09338703E-08  | -0.03927773E-10 | 0.12870404E+05 | 0.12138195E+02  |
| 1000-5000K   | 0.07190480E+02 | 0.06484077E-01 | -0.06428064E-05 | -0.02347879E-08 | 0.03880877E-12  | 0.10674549E+05 | -0.14780892E+02 |



Source: RECALC. OF BURCAT FIT (TSIV TABLES), H298=28 PER MILLER

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2H6

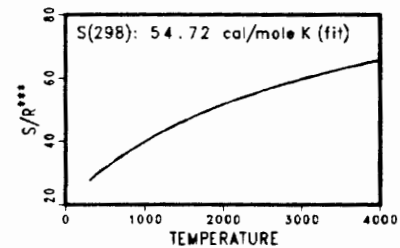
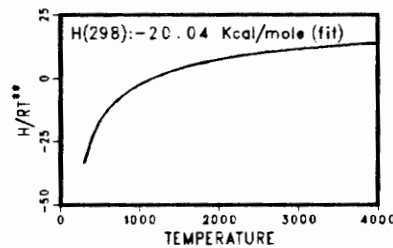
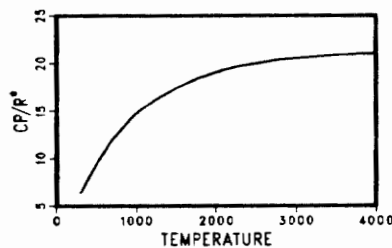
ETHANE

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.14625388E+01 | 0.15494667E-01 | 0.05780507E-04  | -0.12578319E-07 | 0.04586267E-10  | -0.11239176E+05 | 0.14432295E+02  |
| 1000-4000K   | 0.04825938E+02 | 0.13840429E-01 | -0.04557258E-04 | 0.06724967E-08  | -0.03598161E-12 | -0.12717793E+05 | -0.05239506E+02 |



Source: BURCAT (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2HCL

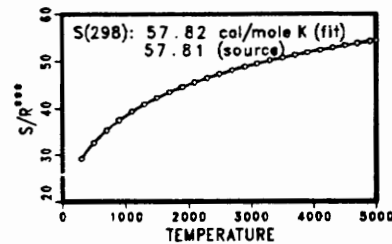
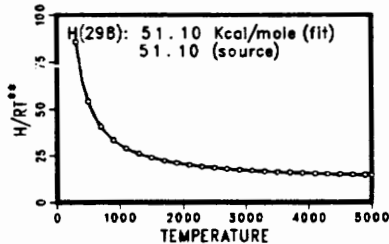
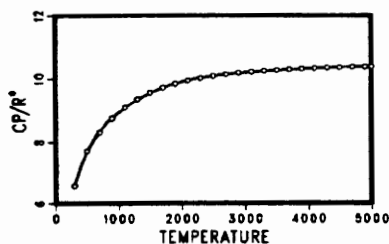
CHLOROACETYLENE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03618443E+02 | 0.13319791E-01 | -0.13218222E-04 | 0.06092023E-07 | -0.08879026E-11 | 0.02415385E+06 | 0.05050645E+02  |
| 1000-5000K   | 0.06295372E+02 | 0.03883113E-01 | -0.15060494E-05 | 0.02700003E-08 | -0.01830213E-12 | 0.02357278E+06 | -0.08137063E+02 |



Source: SNLL FIT TO JANNAF DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2N

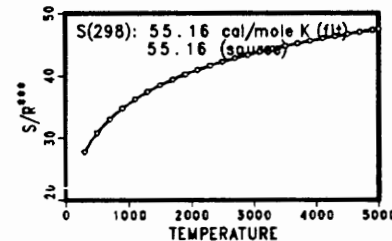
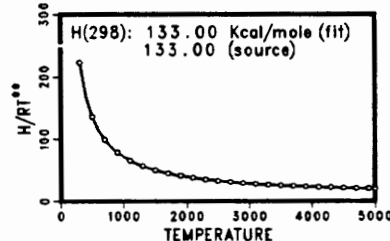
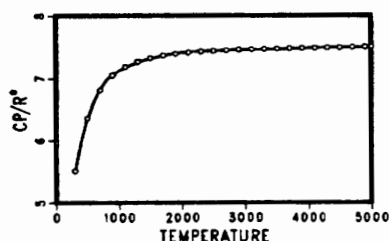
CNC RADICAL

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03498544E+02 | 0.08554433E-01 | -0.06288697E-04 | 0.08638478E-08 | 0.04915996E-11  | 0.06556611E+06 | 0.05548374E+02  |
| 1000-5000K   | 0.06151561E+02 | 0.15116498E-02 | -0.06629362E-05 | 0.12861485E-09 | -0.09160830E-13 | 0.06484318E+06 | -0.08177850E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2N2

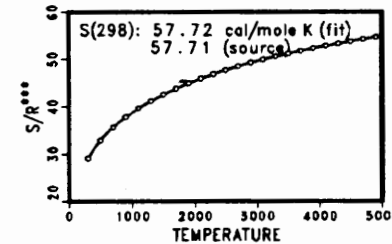
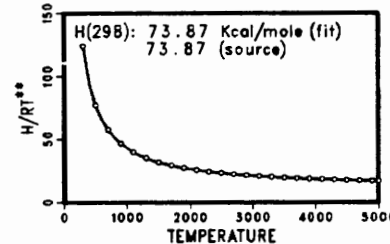
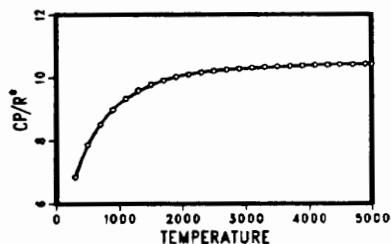
CYANOGEN

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04265459E+02 | 0.11922569E-01 | -0.13420142E-04 | 0.09192297E-07 | -0.02778941E-10 | 0.03547887E+06 | 0.01713212E+02  |
| 1000-5000K   | 0.06548002E+02 | 0.03984707E-01 | -0.16342164E-05 | 0.03038596E-08 | -0.02111069E-12 | 0.03490716E+06 | -0.09735790E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2O

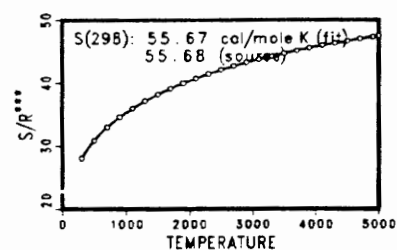
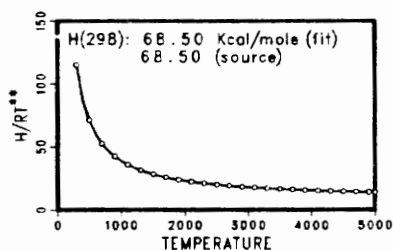
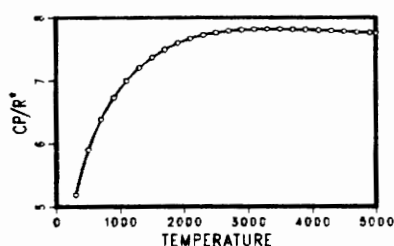
CCO RADICAL

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03368850E+02 | 0.08241803E-01 | -0.08765145E-04 | 0.05569262E-07 | -0.15400086E-11 | 0.03317081E+06 | 0.06713314E+02  |
| 1000-5000K   | 0.04849809E+02 | 0.02947585E-01 | -0.10907286E-05 | 0.01792562E-08 | -0.11157585E-13 | 0.03282055E+06 | -0.06453225E+01 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3

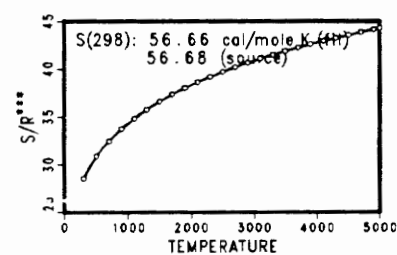
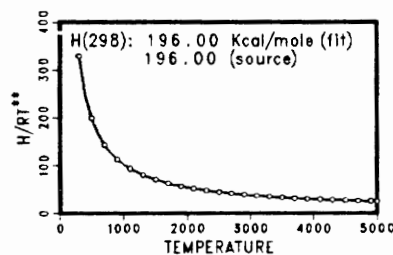
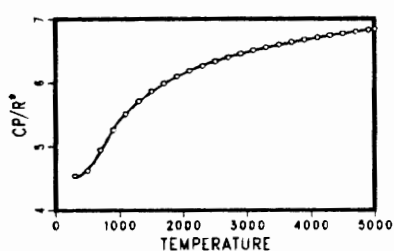
CARBON, TRIATOMIC

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.04345527E+02 | 0.12644661E-02 | -0.04652557E-04 | 0.08695855E-07 | -0.04243535E-10 | 0.09731403E+06 | 0.03519437E+02 |
| 1000-5000K   | 0.03803709E+02 | 0.02253566E-01 | -0.07704534E-05 | 0.13162939E-09 | -0.08694264E-13 | 0.09736135E+06 | 0.06128062E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H2

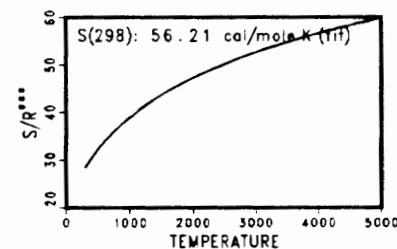
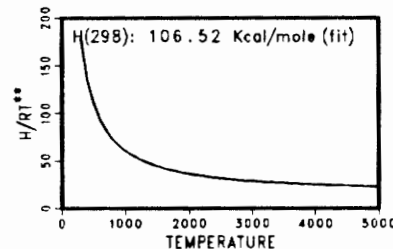
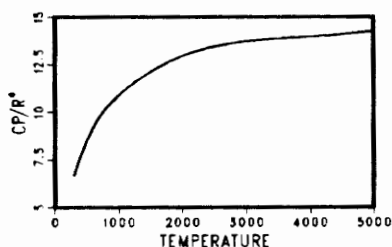
C3H2 RAD

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02691077E+02 | 0.14803664E-01 | -0.03250551E-04 | -0.08644363E-07 | 0.05284877E-10  | 0.05219072E+06 | 0.08757391E+02  |
| 1000-5000K   | 0.06530853E+02 | 0.05870316E-01 | -0.01720776E-04 | 0.02127498E-08  | -0.08291910E-13 | 0.05115213E+06 | -0.11227278E+02 |



Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H4

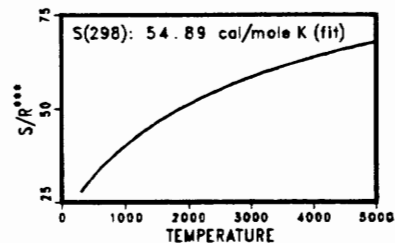
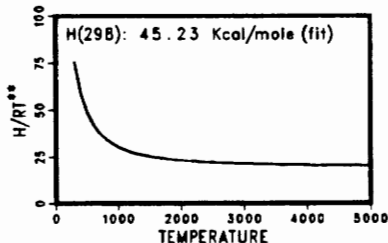
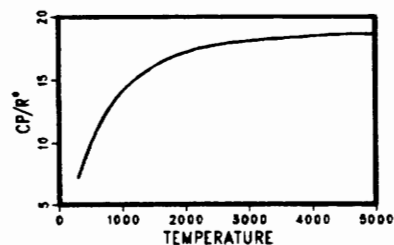
ALLENE

GAS

As of: 4/06/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | -0.02131968E+01 | 0.03358713E+00 | -0.03804870E-03 | 0.02745838E-06 | -0.08690044E-10 | 0.02162048E+06 | 0.02029392E+03  |
| 1000-5000K   | 0.05729144E+02  | 0.12368045E-01 | -0.04805626E-04 | 0.08601364E-08 | -0.05812802E-12 | 0.02012984E+06 | -0.09448668E+02 |



Source: SNLL FIT TO BURCAT VIBRATIONAL FREQUENCIES  
 Comments: (ERROR IN BURCAT COEFFICIENTS)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H4C

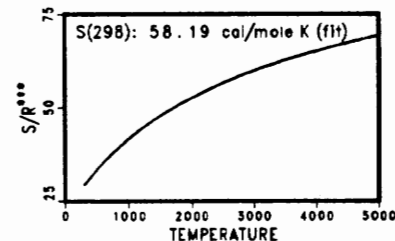
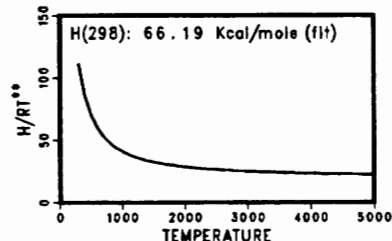
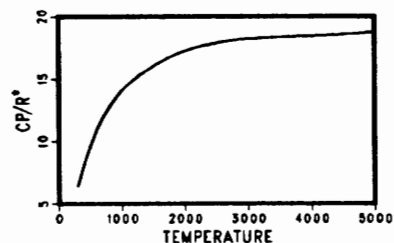
CYCLOPROPENE

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | -0.02462104E+00 | 0.02319721E+00 | -0.01847435E-04 | -0.15927594E-07 | 0.08684615E-10  | 0.03233413E+06 | 0.02271659E+03  |
| 1000-5000K   | 0.06699993E+02  | 0.10357372E-01 | -0.03455116E-04 | 0.05065295E-08  | -0.02668227E-12 | 0.03019905E+06 | -0.13391933E+02 |



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H4P

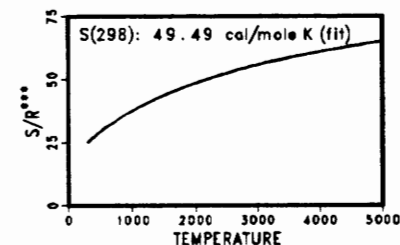
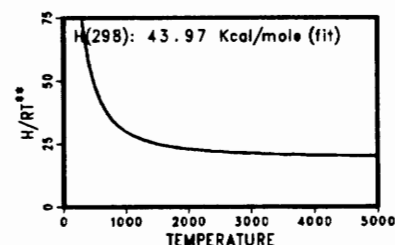
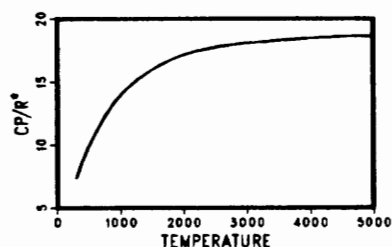
PROPYLENE

GAS

As of: 4/06/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.06271447E+01 | 0.03116179E+00 | -0.03747663E-03 | 0.02964117E-06 | -0.09987381E-10 | 0.02083492E+06 | 0.13468796E+02  |
| 1000-5000K   | 0.05511034E+02 | 0.12469562E-01 | -0.04814164E-04 | 0.08573770E-08 | -0.05771561E-12 | 0.01961967E+06 | -0.10794748E+02 |



Source: SNLL FIT TO BURCAT VIBRATIONAL FREQUENCIES  
 Comments: (ERROR IN BURCAT COEFFICIENTS)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H6

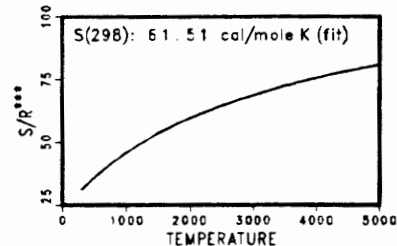
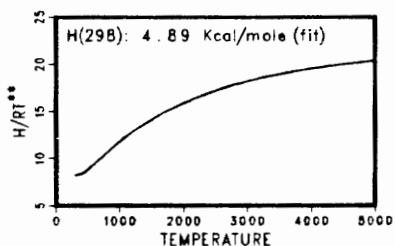
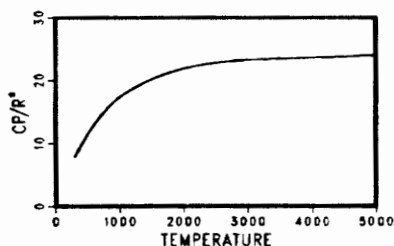
PROPYLENE

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.14933071E+01 | 0.02092517E+00 | 0.04486794E-04  | -0.16689121E-07 | 0.07158146E-10  | 0.10748264E+04  | 0.16145340E+02  |
| 1000-5000K   | 0.06732257E+02 | 0.14908336E-01 | -0.04949899E-04 | 0.07212022E-08  | -0.03766204E-12 | -0.09235703E+04 | -0.13313348E+02 |



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H8

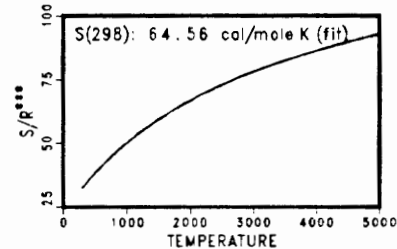
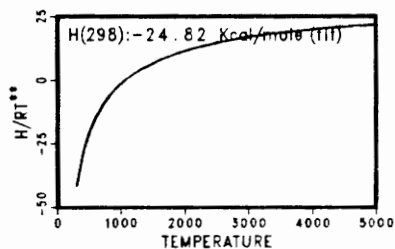
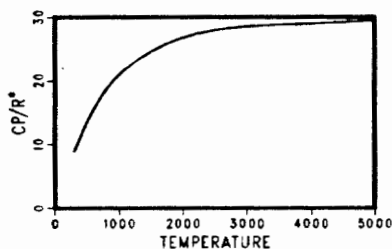
PROPANE

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.08969208E+01 | 0.02668986E+00 | 0.05431425E-04  | -0.02126000E-06 | 0.09243330E-10  | -0.13954918E+05 | 0.01935533E+03  |
| 1000-5000K   | 0.07525217E+02 | 0.01889034E+00 | -0.06283924E-04 | 0.09179373E-08  | -0.04812410E-12 | -0.16464548E+05 | -0.01784390E+03 |



Source: BURCAT (NASA LEWIS TABLES)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3O2

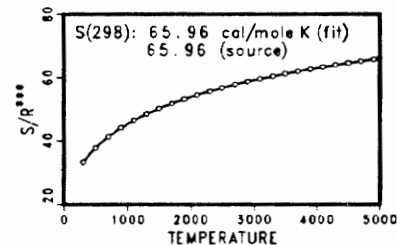
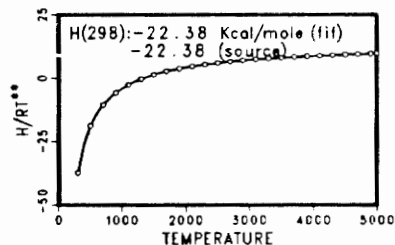
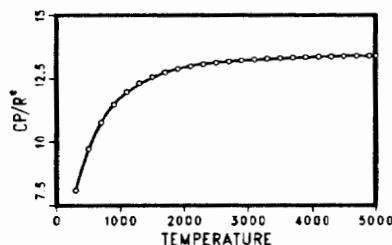
CARBON SUBOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.04018127E+02 | 0.01836660E+00 | -0.01907148E-03 | 0.11855871E-07 | -0.03418747E-10 | -0.13128236E+05 | 0.05582083E+02  |
| 1000-5000K   | 0.08098897E+02 | 0.05560039E-01 | -0.02312264E-04 | 0.04340709E-08 | -0.03036387E-12 | -0.14214353E+05 | -0.15219745E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C4

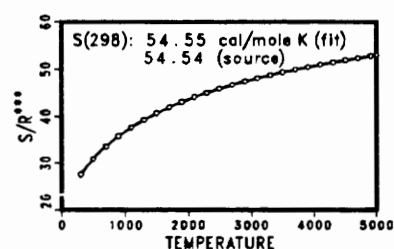
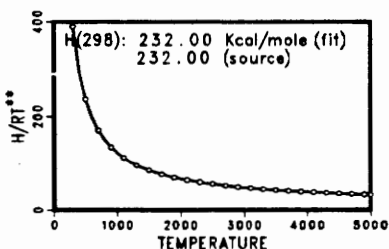
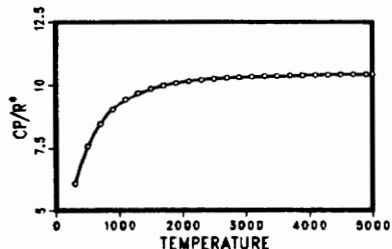
CARBON, TETRATOMIC

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02343028E+02 | 0.16429811E-01 | -0.15279858E-04 | 0.07343826E-07 | -0.15822743E-11 | 0.11545384E+06 | 0.09826204E+02  |
| 1000-5000K   | 0.06500180E+02 | 0.04228632E-01 | -0.01790717E-04 | 0.03404812E-08 | -0.02403978E-12 | 0.11434008E+06 | -0.11488894E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: C4H

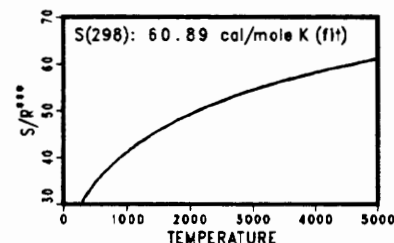
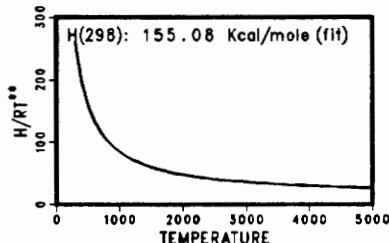
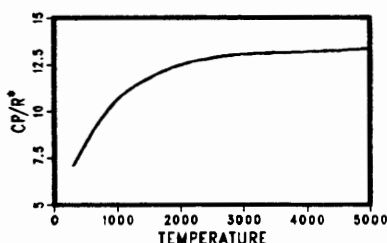
C4H RAD

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.05023247E+02 | 0.07092375E-01 | -0.06073762E-07 | -0.02275752E-07 | 0.08086994E-11  | 0.07623812E+06 | -0.06942594E+00 |
| 1000-5000K   | 0.06242882E+02 | 0.06193682E-01 | -0.02085931E-04 | 0.03082203E-08  | -0.16364826E-13 | 0.07568019E+06 | -0.07210806E+02 |



Source: BURCAT (TECHNION REPORTS)

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: C4H2

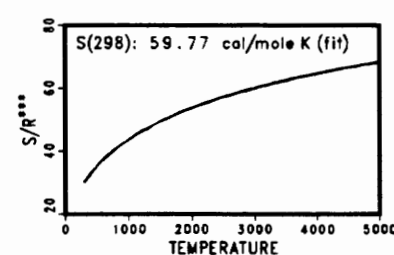
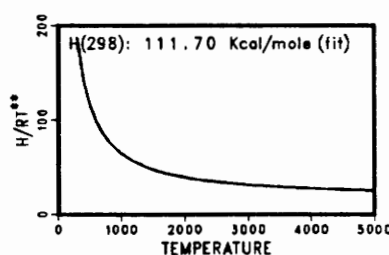
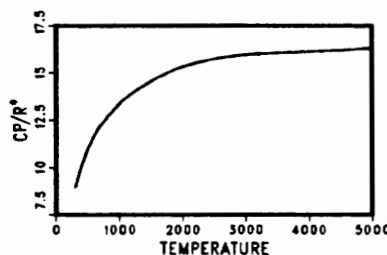
BUTADIYNE

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04005191E+02 | 0.01981000E+00 | -0.09865877E-04 | -0.06635158E-07 | 0.06077413E-10  | 0.05424065E+06 | 0.01845736E+02  |
| 1000-5000K   | 0.09031407E+02 | 0.06047252E-01 | -0.01948788E-04 | 0.02754863E-08  | -0.13856080E-13 | 0.05294735E+06 | -0.02385067E+03 |



Source: BURCAT (LSU CALCULATIONS)

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

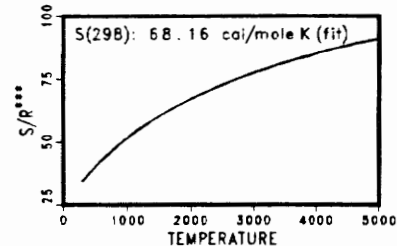
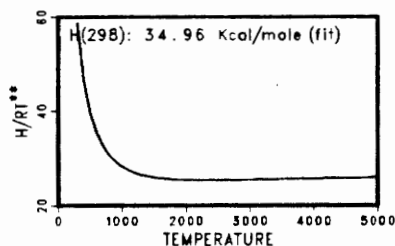
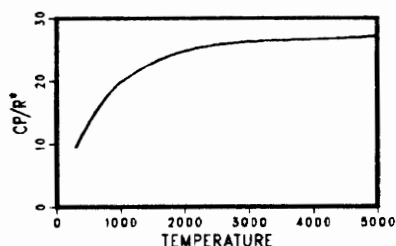
Species: C4H6

2-BUTAYN (DIMETHYLACETYLENE) GAS

As of: 12/01/86

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K | 0.03197108E+02 | 0.02025591E+00 | 0.06510192E-04  | -0.16584423E-07 | 0.06400282E-10  | 0.15715203E+05 | 0.09895660E+02  |
| 1000-5000K | 0.08046583E+02 | 0.16485251E-01 | -0.05522227E-04 | 0.08123593E-08  | -0.04295078E-12 | 0.13701305E+05 | -0.01800457E+03 |



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C4H8

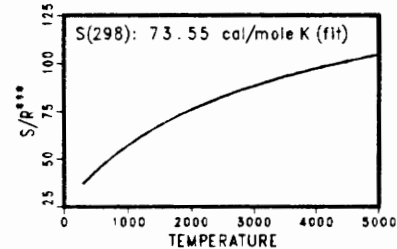
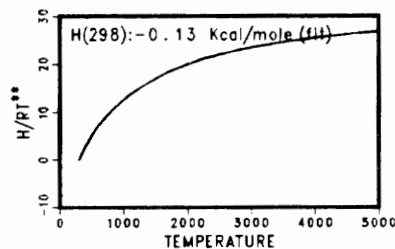
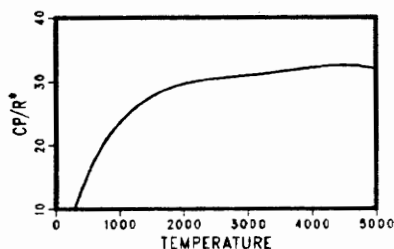
1-BUTENE

GAS

As of: 12/03/86

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 0300-1000K | 0.11811380E+01 | 0.03085338E+00 | 0.05086524E-04  | -0.02465488E-06 | 0.11110192E-10  | -0.01790400E+05 | 0.02106247E+03 |
| 1000-5000K | 0.02053584E+02 | 0.03435050E+00 | -0.15883196E-04 | 0.03308966E-07  | -0.02536104E-11 | -0.02139723E+05 | 0.15543201E+02 |



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C5

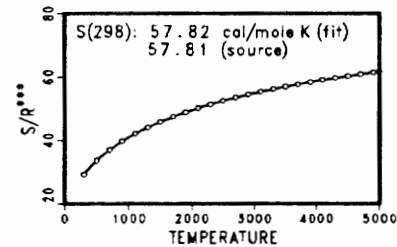
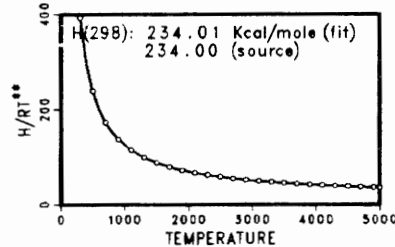
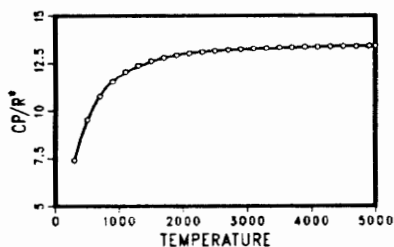
CARBON, PENTATOMIC

GAS

As of: 12/12/86

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K | 0.02115273E+02 | 0.02326331E+00 | -0.02109499E-03 | 0.09072734E-07 | -0.15400926E-11 | 0.11627381E+06 | 0.10976027E+02  |
| 1000-5000K | 0.08078081E+02 | 0.05743464E-01 | -0.02436405E-04 | 0.04638916E-08 | -0.03278909E-12 | 0.11470216E+06 | -0.01953023E+03 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C5H

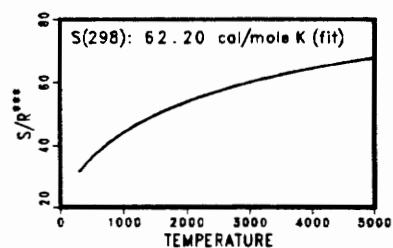
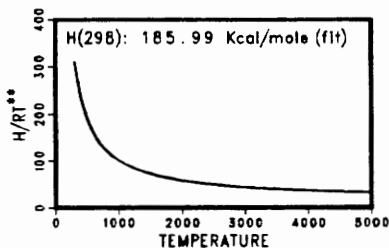
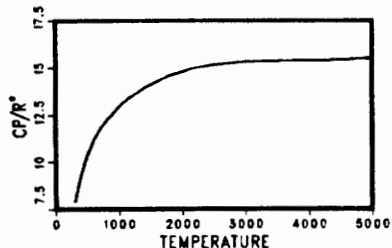
C5H RAD

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.16348248E+01 | 0.02509538E+00 | -0.12066364E-04 | -0.10465110E-07 | 0.08809988E-10  | 0.09212488E+06 | 0.15121937E+02  |
| 1000-5000K   | 0.08695749E+02 | 0.06054301E-01 | -0.02016010E-04 | 0.02892892E-08  | -0.14700996E-13 | 0.09031069E+06 | -0.02101594E+03 |



Source: BURCAT FIT (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C5H12

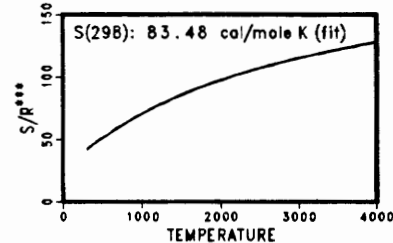
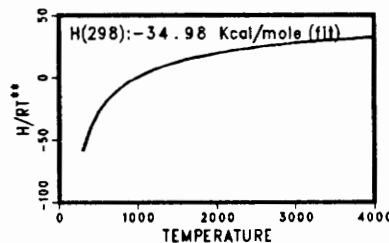
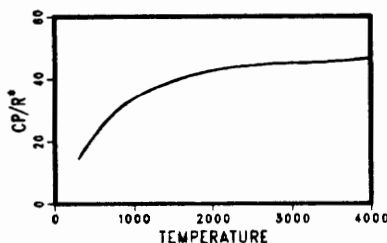
N-PENTANE

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.01877907E+02 | 0.04121645E+00 | 0.12532337E-04  | -0.03701536E-06 | 0.15255685E-10 | -0.02003815E+06 | 0.01877256E+03  |
| 1000-4000K   | 0.16677979E+02 | 0.02114483E+00 | -0.03533321E-04 | -0.05742202E-08 | 0.15159483E-12 | -0.02553670E+06 | -0.06372940E+03 |



Source: BURCAT FIT (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C5H2

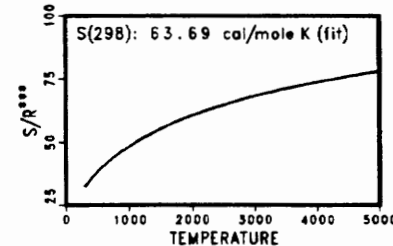
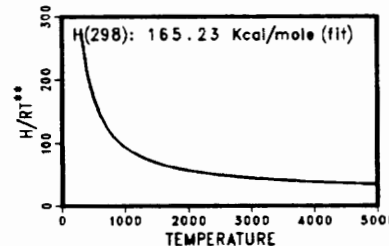
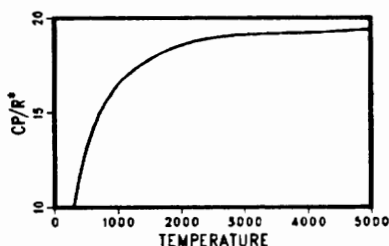
C5H2 RAD

GAS

As of: 2/05/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03062321E+02 | 0.02709998E+00 | -0.10091697E-04 | -0.12727451E-07 | 0.09167219E-10  | 0.08114969E+06 | 0.07071078E+02  |
| 1000-5000K   | 0.11329175E+02 | 0.07424056E-01 | -0.02628188E-04 | 0.04082541E-08  | -0.02301332E-12 | 0.07878706E+06 | -0.03617117E+03 |



Source: BURCAT FIT (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



Species: C5H3

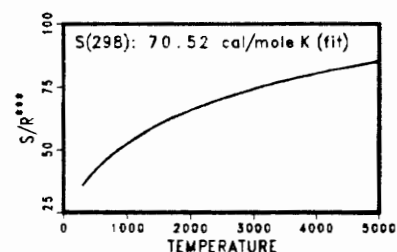
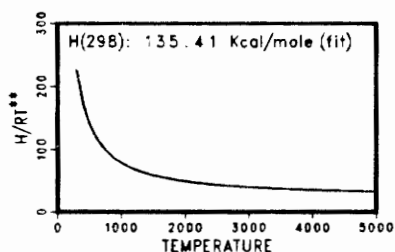
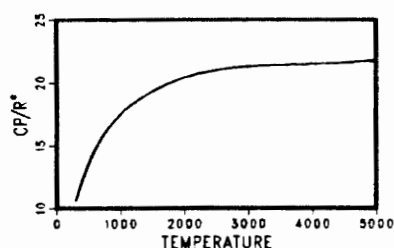
C5H3 RAD

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04328720E+02 | 0.02352480E+00 | -0.05856723E-04 | -0.12154494E-07 | 0.07726478E-10  | 0.06588531E+06 | 0.04173258E+02  |
| 1000-5000K   | 0.10787622E+02 | 0.09539619E-01 | -0.03206744E-04 | 0.04733323E-08  | -0.02512135E-12 | 0.06392904E+06 | -0.03005444E+03 |



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C5H6

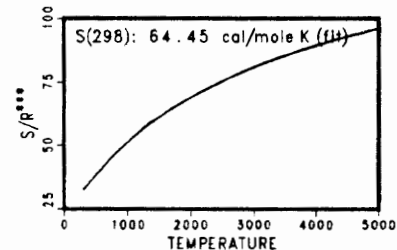
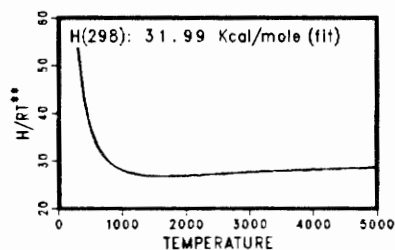
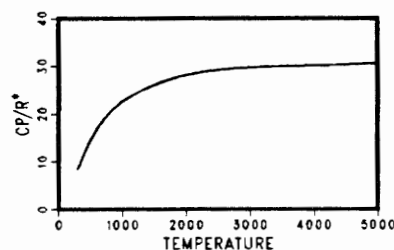
CYCLOPENTADIENE

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | -0.03196739E+02 | 0.04081361E+00 | 0.06816505E-05  | -0.03137459E-06 | 0.15772230E-10  | 0.15290676E+05 | 0.03869938E+03  |
| 1000-5000K   | 0.09689815E+02  | 0.01838262E+00 | -0.06264884E-04 | 0.09393377E-08  | -0.05087708E-12 | 0.11021242E+05 | -0.03122908E+03 |



Source: BURCAT FIT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C6H

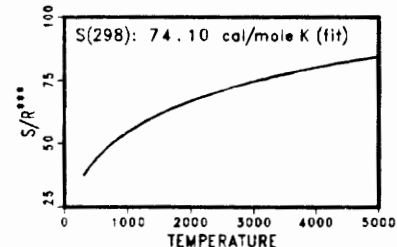
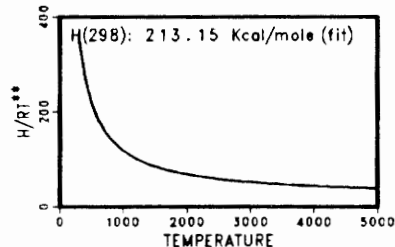
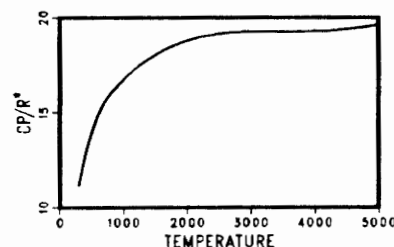
C6H RAD

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04769848E+02 | 0.02457279E+00 | -0.07561252E-04 | -0.14806908E-07 | 0.09768053E-10  | 0.10485231E+06 | 0.03241530E+02  |
| 1000-5000K   | 0.11587352E+02 | 0.07295362E-01 | -0.02466008E-04 | 0.03407045E-08  | -0.14981855E-13 | 0.10314481E+06 | -0.03172578E+03 |



Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C6H10

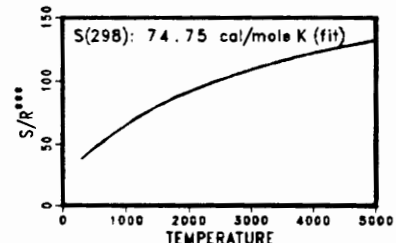
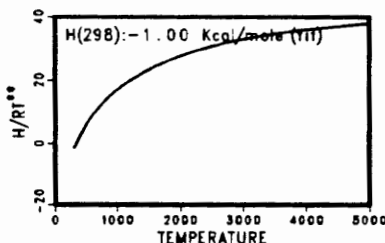
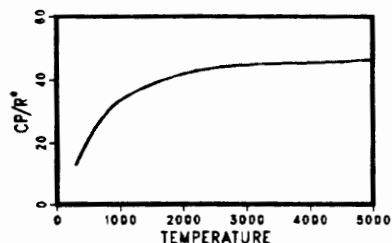
CYCLOHEXENE

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | -0.13942280E+01 | 0.04720693E+00 | 0.11960419E-04  | -0.04162895E-06 | 0.01740335E-09  | -0.02217790E+05 | 0.03129603E+03  |
| 1000-5000K   | 0.15927771E+02  | 0.02374412E+00 | -0.06908672E-04 | 0.08109777E-08  | -0.02683122E-12 | -0.08642656E+05 | -0.06525186E+03 |



Source: BURCAT FIT (LSU CALCULATIONS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C6H14

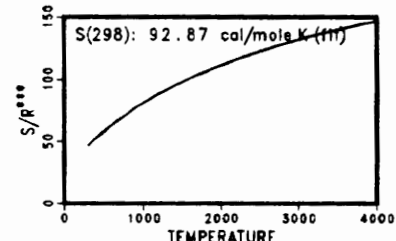
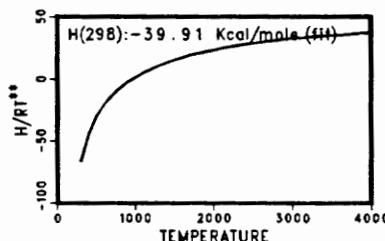
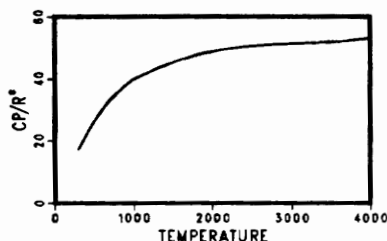
N-HEXANE

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.01836174E+02 | 0.05098461E+00 | 0.12595857E-04  | -0.04428362E-06 | 0.01872237E-09 | -0.02292749E+06 | 0.02088145E+03  |
| 1000-4000K   | 0.02280471E+03 | 0.02097989E+00 | -0.03530674E-04 | -0.05466245E-08 | 0.14789499E-12 | -0.03073756E+06 | -0.09583162E+03 |



Source: BURCAT FIT (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C6H2

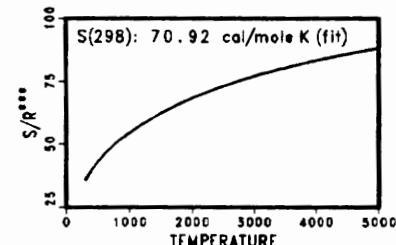
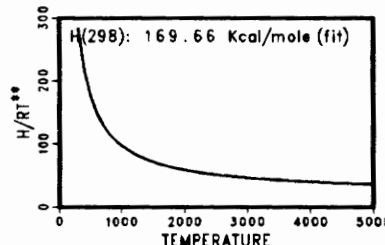
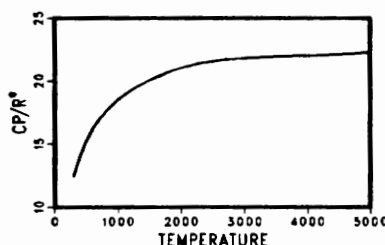
HEXATRIYNE

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.05751085E+02 | 0.02636719E+00 | -0.11667596E-04 | -0.10714498E-07 | 0.08790297E-10  | 0.08262012E+06 | -0.04335532E+02 |
| 1000-5000K   | 0.12756519E+02 | 0.08034381E-01 | -0.02618215E-04 | 0.03725060E-08  | -0.01878850E-12 | 0.08075469E+06 | -0.04041262E+03 |



Source: BURCAT (LSU CALCULATIONS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C6H3

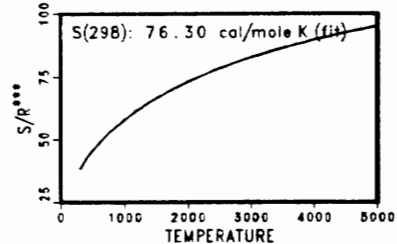
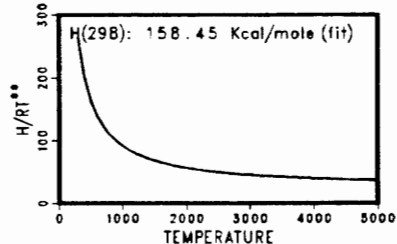
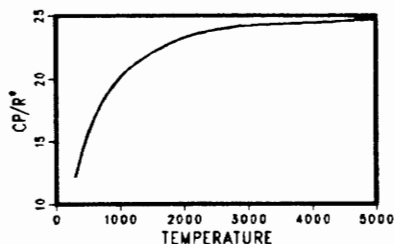
C6H3 RAD

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.05007089E+02 | 0.02692851E+00 | -0.05919865E-04 | -0.15272335E-07 | 0.09408310E-10  | 0.07713200E+06 | 0.02225621E+02  |
| 1000-5000K   | 0.12761181E+02 | 0.10385573E-01 | -0.03479192E-04 | 0.05109733E-08  | -0.02690965E-12 | 0.07477706E+06 | -0.03891745E+03 |



Source: BURCAT FIT (LSU CALCULATIONS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C6H4

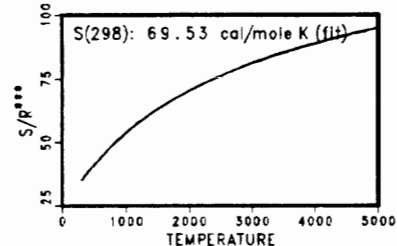
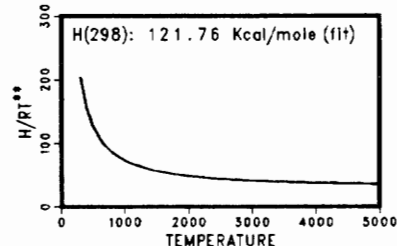
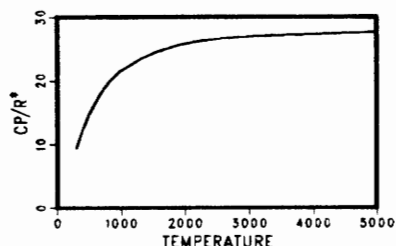
BENZYNE

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | -0.13004846E+01 | 0.03866476E+00 | -0.03643944E-04 | -0.02668580E-06 | 0.14509357E-10  | 0.06002907E+06 | 0.03124939E+03  |
| 1000-5000K   | 0.10062741E+02  | 0.01690304E+00 | -0.06473045E-04 | 0.11240806E-08  | -0.07307566E-12 | 0.05645373E+06 | -0.02969310E+03 |



Source: BURCAT FIT (LSU CALCULATIONS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C6H5

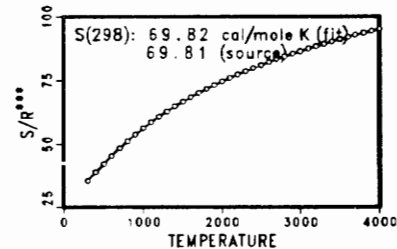
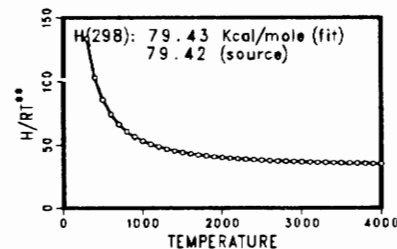
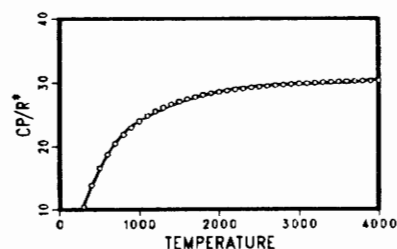
PHENYL

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.11435567E+00 | 0.03627324E+00 | 0.11582856E-05  | -0.02196964E-06 | 0.08463556E-10 | 0.03836054E+06 | 0.02380117E+03  |
| 1000-4000K   | 0.15775887E+02 | 0.09651109E-01 | -0.09429416E-05 | -0.05469111E-08 | 0.10265216E-12 | 0.03302698E+06 | -0.06176280E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

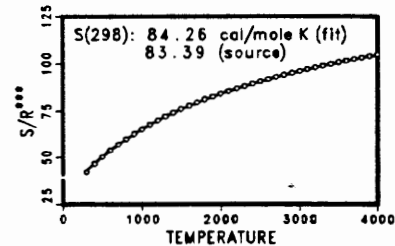
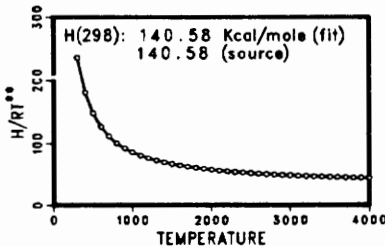
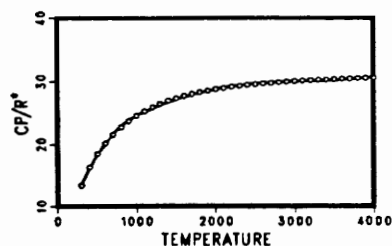
Species: C6H5(L)

HCCCHCHCHCH CCCCCIS HCCH CIS 2A' GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.04854268E+02 | 0.03031659E+00 | 0.01742892E-05  | -0.01811010E-06 | 0.07392511E-10 | 0.06798733E+06 | 0.05854934E+02  |
| 1000-4000K   | 0.01721540E+03 | 0.08621068E-01 | -0.08221340E-05 | -0.04752164E-08 | 0.08844086E-12 | 0.06385819E+06 | -0.06139128E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C6H5O

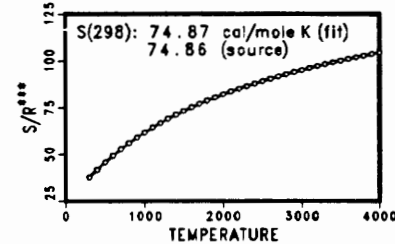
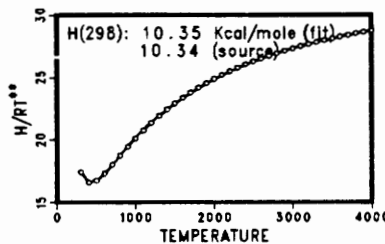
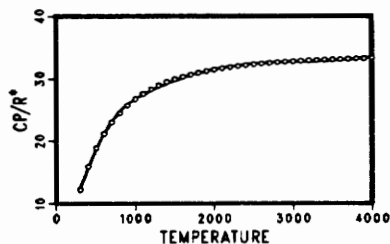
PHENOXY

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.11074965E+01 | 0.03956945E+00 | 0.08497295E-05  | -0.02436311E-06 | 0.09650659E-10 | 0.03159672E+05  | 0.01973496E+03  |
| 1000-4000K   | 0.01822638E+03 | 0.10039851E-01 | -0.09915668E-05 | -0.05672804E-08 | 0.10683716E-12 | -0.02620846E+05 | -0.07361390E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

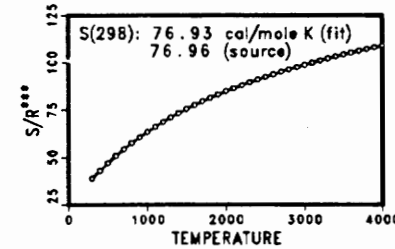
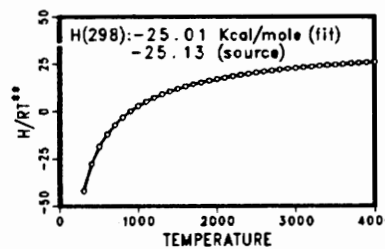
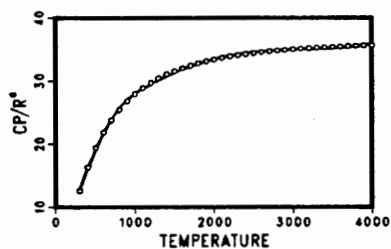
Species: C6H5OH

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.13914556E+01 | 0.03931957E+00 | 0.01777096E-04  | -0.02277673E-06 | 0.08309659E-10 | -0.14721809E+05 | 0.01917813E+03  |
| 1000-4000K   | 0.01821632E+03 | 0.11424269E-01 | -0.10966843E-05 | -0.06427442E-08 | 0.11988930E-12 | -0.02053664E+06 | -0.07304233E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C6H6

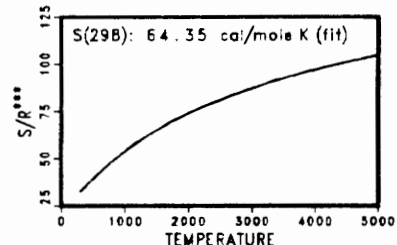
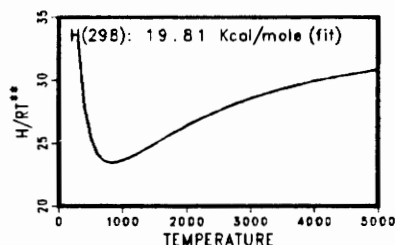
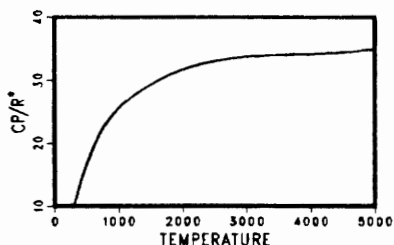
BENZENE

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | -0.03138012E+02 | 0.04723103E+00 | -0.02962207E-04 | -0.03262819E-06 | 0.01718691E-09  | 0.08890031E+05 | 0.03657573E+03  |
| 1000-5000K   | 0.12910740E+02  | 0.01723296E+00 | -0.05024210E-04 | 0.05893497E-08  | -0.01947521E-12 | 0.03664511E+05 | -0.05002699E+03 |



Source: BURCAT FIT (LSU CALCULATIONS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C6H7

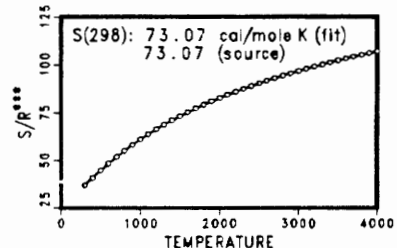
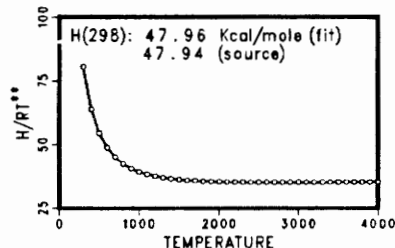
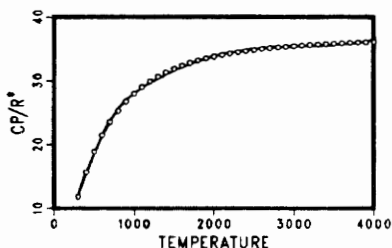
BENZYL 2B1

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.04639166E+01 | 0.03975928E+00 | 0.02529095E-04  | -0.02223792E-06 | 0.07557053E-10 | 0.02225169E+06 | 0.02235387E+03  |
| 1000-4000K   | 0.01755221E+03 | 0.12270795E-01 | -0.11857424E-05 | -0.06959661E-08 | 0.13013259E-12 | 0.16245813E+05 | -0.07166588E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C8H

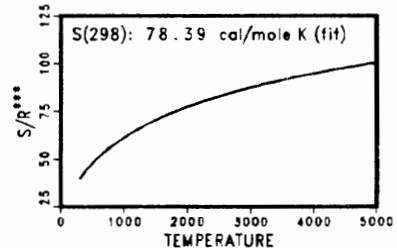
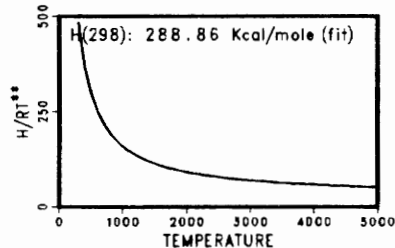
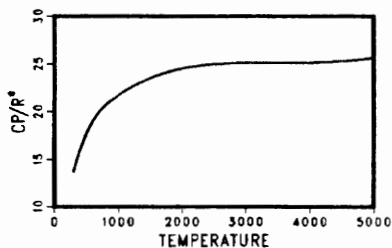
C8H RAD

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04489507E+02 | 0.03521521E+00 | -0.10193898E-04 | -0.02197024E-06 | 0.14214164E-10  | 0.14259919E+06 | 0.03996225E+02  |
| 1000-5000K   | 0.14749907E+02 | 0.09931501E-01 | -0.03374841E-04 | 0.04687592E-08  | -0.02073536E-12 | 0.13994481E+06 | -0.04892689E+03 |



Source: BURCAT (LSU CALCULATIONS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C8H2

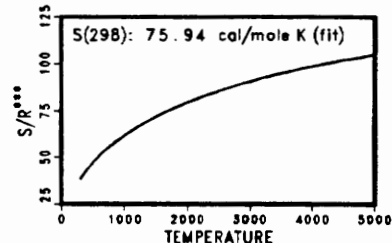
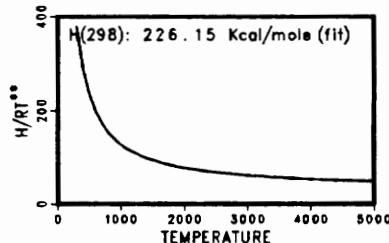
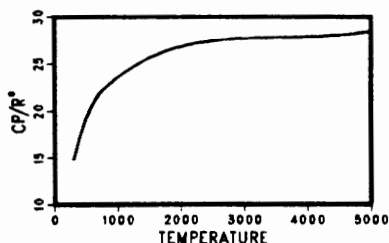
OCTATETRAYNE

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04630427E+02 | 0.03937080E+00 | -0.11480348E-04 | -0.02562213E-06 | 0.16707913E-10  | 0.11082850E+06 | 0.08077425E+01  |
| 1000-5000K   | 0.15680213E+02 | 0.11154614E-01 | -0.03724372E-04 | 0.05197891E-08  | -0.02375550E-12 | 0.10811225E+06 | -0.05571437E+03 |



Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CCL

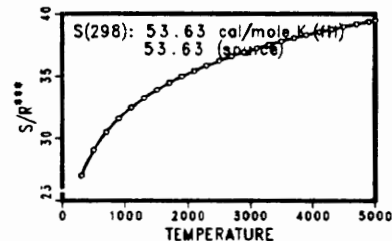
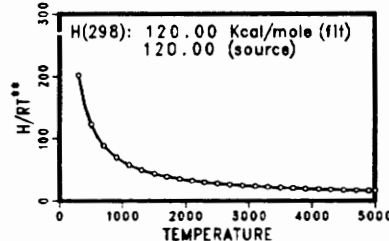
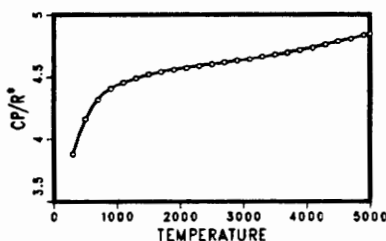
CARBON MONOCHLORIDE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03188782E+02 | 0.02965197E-01 | -0.02305370E-04 | 0.04866913E-08 | 0.09990141E-12  | 0.05932937E+06 | 0.08037628E+02 |
| 1000-5000K   | 0.04072804E+02 | 0.05508787E-02 | -0.02319334E-05 | 0.04669038E-09 | -0.03236856E-13 | 0.05909198E+06 | 0.03481073E+02 |



Source: SNLL FIT TO JANNAF DATA

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CCL2

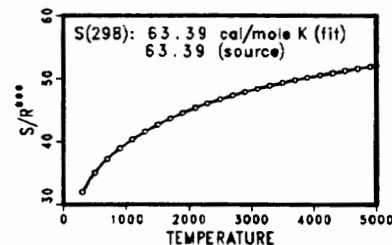
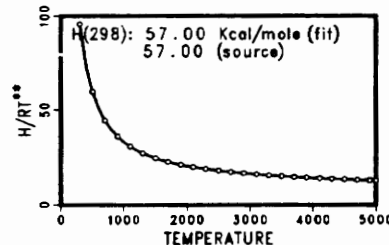
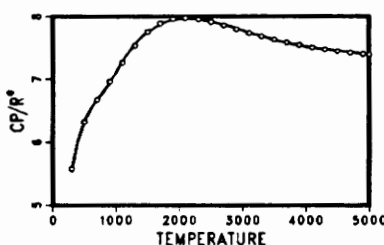
CARBON DICHLORIDE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02651916E+02 | 0.15169552E-01 | -0.02230162E-03 | 0.15041039E-07 | -0.03452951E-10 | 0.02739027E+06 | 0.13136703E+02 |
| 1000-5000K   | 0.03501741E+02 | 0.05749397E-01 | -0.02589721E-04 | 0.04783950E-08 | -0.03188271E-12 | 0.02763633E+06 | 0.10829469E+02 |



Source: SNLL FIT TO JANNAF DATA

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CCL3

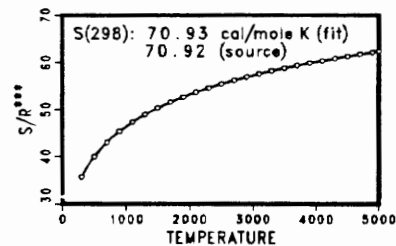
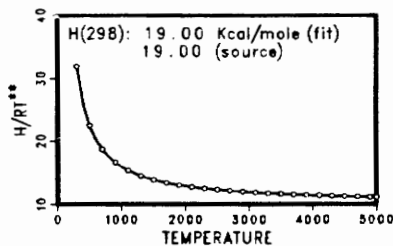
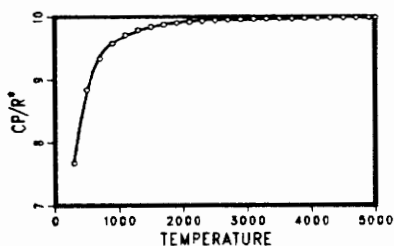
TRICHLOROMETHYL

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04866162E+02 | 0.11903691E-01 | -0.07849049E-04 | -0.14484371E-08 | 0.02169760E-10  | 0.07655364E+05 | 0.04781636E+02  |
| 1000-5000K   | 0.08639372E+02 | 0.15880909E-02 | -0.07176410E-05 | 0.14271238E-09  | -0.10407368E-13 | 0.06701065E+05 | -0.14518221E+02 |



Source: SNLL FIT TO JANNAF DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CCL4

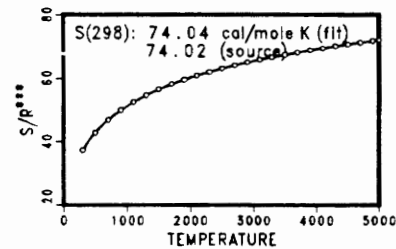
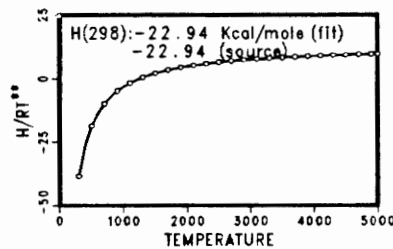
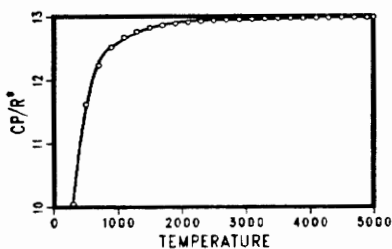
CARBON TETRACHLORIDE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.06286815E+02 | 0.15997799E-01 | -0.10203526E-04 | -0.03043311E-07 | 0.03546287E-10  | -0.14032573E+05 | -0.02850812E+02 |
| 1000-5000K   | 0.11369968E+02 | 0.01933276E-01 | -0.08832003E-05 | 0.01770067E-08  | -0.12982896E-13 | -0.15283466E+05 | -0.02874324E+03 |



Source: SNLL FIT TO JANNAF DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH

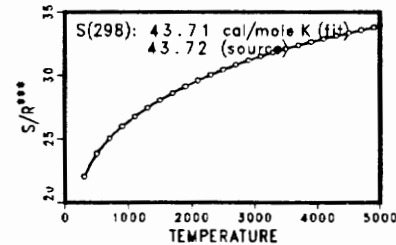
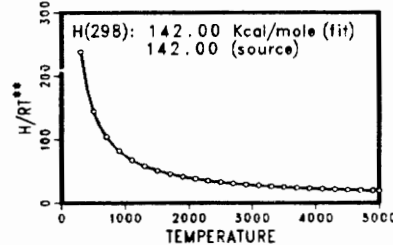
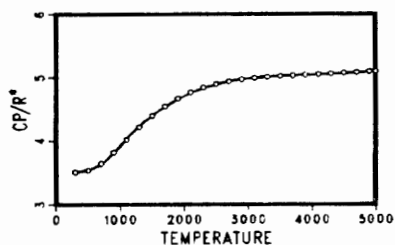
METHYLDIYNE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03200202E+02 | 0.02072875E-01 | -0.05134431E-04 | 0.05733890E-07 | -0.01955533E-10 | 0.07045259E+06 | 0.03331587E+02 |
| 1000-5000K   | 0.02196223E+02 | 0.02340381E-01 | -0.07058201E-05 | 0.09007582E-09 | -0.03855040E-13 | 0.07086723E+06 | 0.09178373E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

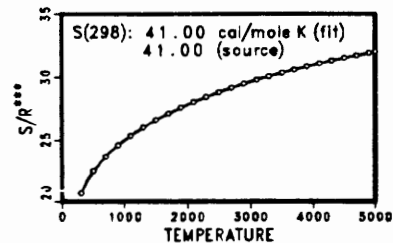
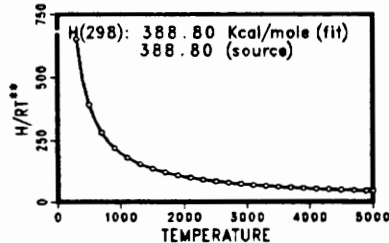
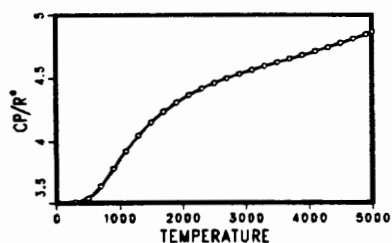
Species: CH<sup>+</sup>

METHYLLIDYNE, UNIPosITIVE ION GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03327207E+02 | 0.13470505E-02 | -0.03895861E-04 | 0.05129390E-07 | -0.02054575E-10 | 0.01946452E+07 | 0.14084738E+01 |
| 1000-5000K   | 0.02753358E+02 | 0.15528998E-02 | -0.05368453E-05 | 0.08921772E-09 | -0.05416801E-13 | 0.01948467E+07 | 0.04654892E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>

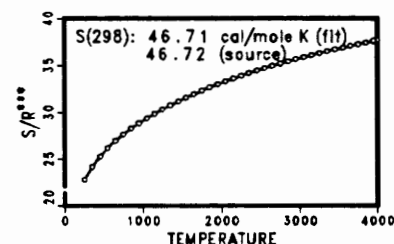
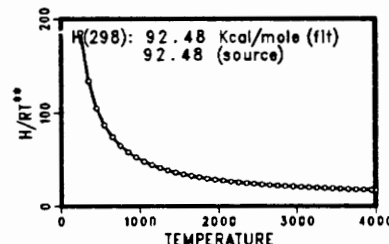
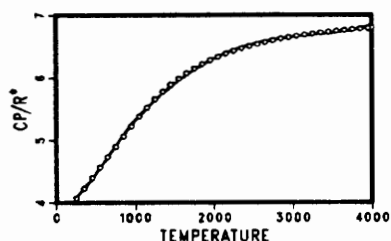
METHYLENE, TRIPLET

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0250-1000K   | 0.03762237E+02 | 0.11598191E-02 | 0.02489585E-05  | 0.08800836E-08  | -0.07332435E-11 | 0.04536790E+06 | 0.01712577E+02 |
| 1000-4000K   | 0.03636407E+02 | 0.01933056E-01 | -0.01687016E-05 | -0.10098994E-09 | 0.01808255E-12  | 0.04534134E+06 | 0.02156560E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>(S)

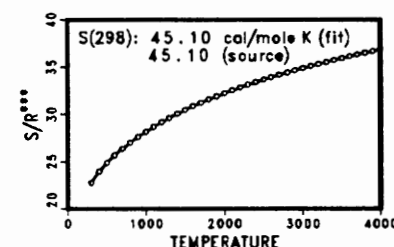
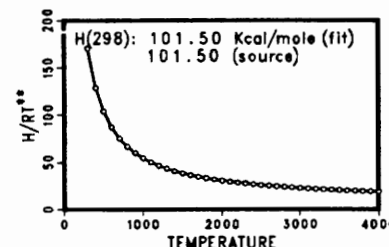
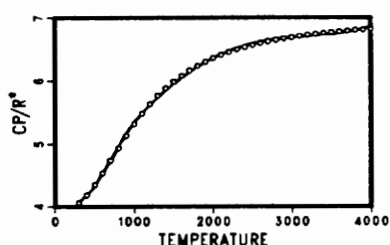
METHYLENE, SINGLET

GAS

As of: 3/12/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03971265E+02 | -0.01699088E-02 | 0.10253689E-05  | 0.02492550E-07  | -0.01981266E-10 | 0.04989367E+06 | 0.05753207E+00 |
| 1000-4000K   | 0.03552888E+02 | 0.02066788E-01  | -0.01914116E-05 | -0.11046733E-09 | 0.02021349E-12  | 0.04984975E+06 | 0.01686570E+02 |



Source: FIT TO BAC-MP4 DATA WITH H298=101.5 PER MILLER

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



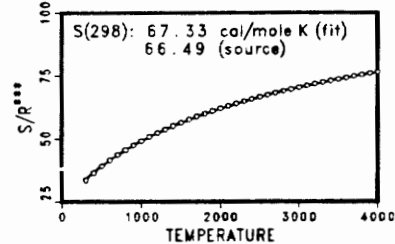
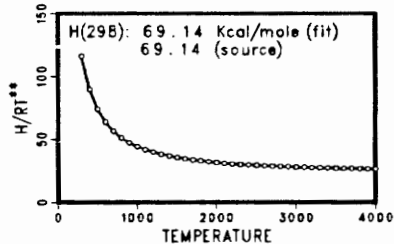
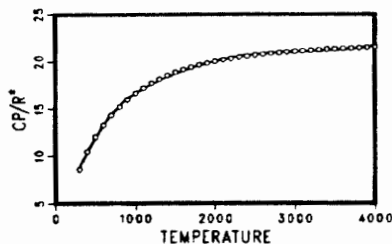
Species: CH<sub>2</sub>CHCCH

BUT-1-YN-3-ENE PLANAR CS GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03233893E+02 | 0.01865634E+00 | 0.12703205E-05  | -0.09410096E-07 | 0.02956110E-10 | 0.03301097E+06 | 0.09922676E+02  |
| 1000-4000K   | 0.10697773E+02 | 0.06982014E-01 | -0.06567747E-05 | -0.03884517E-08 | 0.07200946E-12 | 0.03034803E+06 | -0.03128430E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>CHCCH<sub>2</sub>

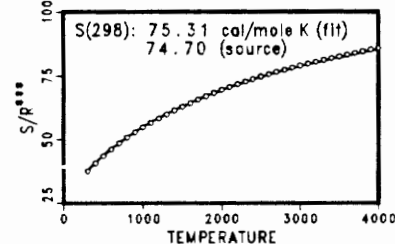
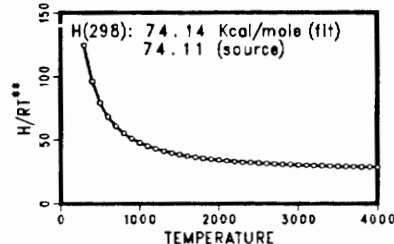
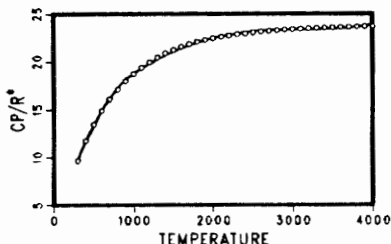
CS

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03879443E+02 | 0.01997663E+00 | 0.01872777E-04  | -0.09306953E-07 | 0.02386116E-10 | 0.03526859E+06 | 0.09842152E+02  |
| 1000-4000K   | 0.11997762E+02 | 0.07990580E-01 | -0.08098172E-05 | -0.04568733E-08 | 0.08636911E-12 | 0.03228493E+06 | -0.03528494E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>CHCH<sub>2</sub>

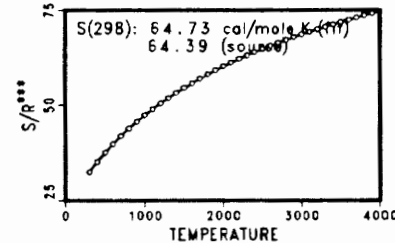
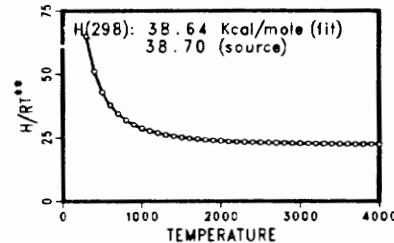
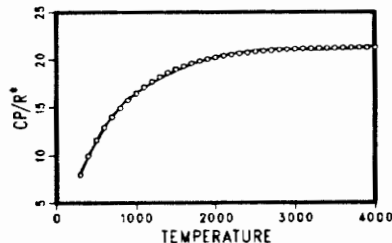
PROP-1-ENYL C2V 2A2

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02276486E+02 | 0.01985564E+00 | 0.11238421E-05  | -0.10145757E-07 | 0.03441342E-10 | 0.01789496E+06 | 0.13725151E+02  |
| 1000-4000K   | 0.09651539E+02 | 0.08075596E-01 | -0.07965424E-05 | -0.04650696E-08 | 0.08603281E-12 | 0.15300955E+05 | -0.02686773E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>CHCHCH

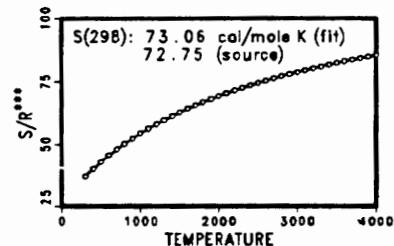
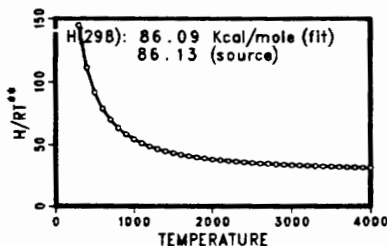
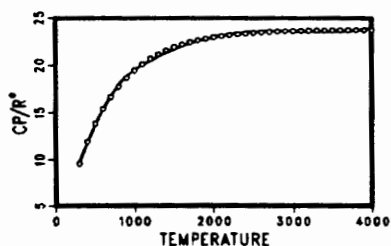
2A' CCCC TRANS HCCH CIS

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02995240E+02 | 0.02288456E+00 | 0.01975471E-04  | -0.11482454E-07 | 0.03197823E-10 | 0.04142218E+06 | 0.12894539E+02  |
| 1000-4000K   | 0.12865971E+02 | 0.07943369E-01 | -0.08626466E-05 | -0.04655635E-08 | 0.08951131E-12 | 0.03783552E+06 | -0.04182502E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>CHCHCH<sub>2</sub>

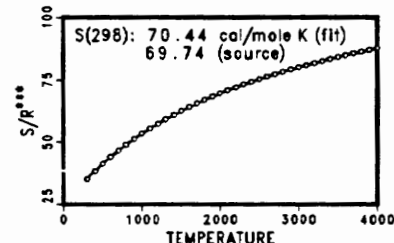
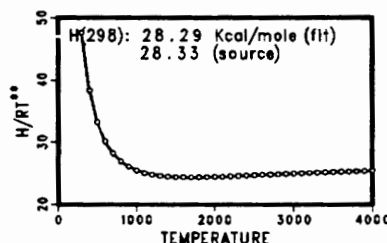
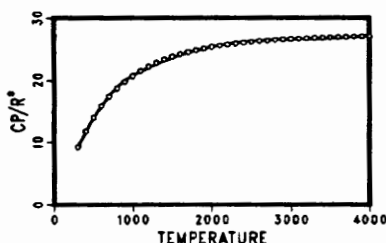
TRANS-1,3-BUTADIENE

GAS

As of: 12/01/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.01931624E+02 | 0.02479030E+00 | 0.03018071E-04  | -0.11546856E-07 | 0.02586623E-10 | 0.12554682E+05 | 0.01701999E+03  |
| 1000-4000K   | 0.12544366E+02 | 0.09596525E-01 | -0.09187012E-05 | -0.05429640E-08 | 0.10053636E-12 | 0.08597330E+05 | -0.04217450E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>CL<sub>2</sub>

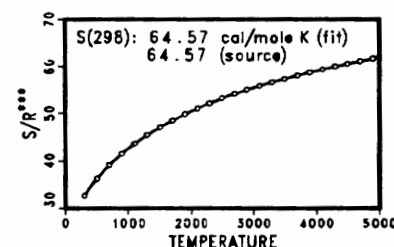
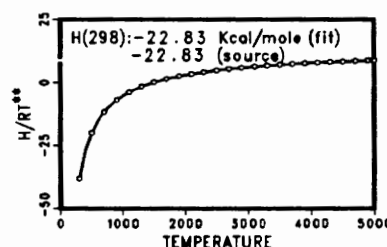
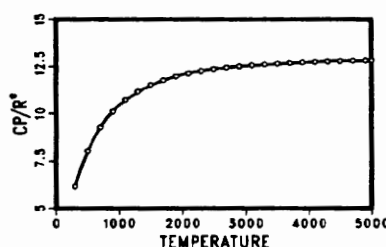
DICHLOROMETHANE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.14232844E+01 | 0.02116658E+00 | -0.02178088E-03 | 0.13458726E-07 | -0.03811649E-10 | -0.12686636E+05 | 0.01893445E+03  |
| 1000-5000K   | 0.05917327E+02 | 0.06762395E-01 | -0.02676163E-04 | 0.04856687E-08 | -0.03316973E-12 | -0.13859256E+05 | -0.03877739E+02 |



Source: SNLL FIT TO JANNAF DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>CO

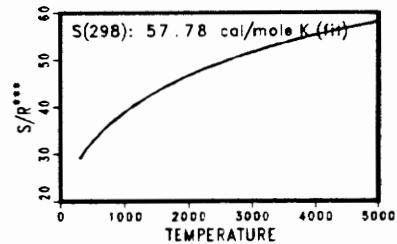
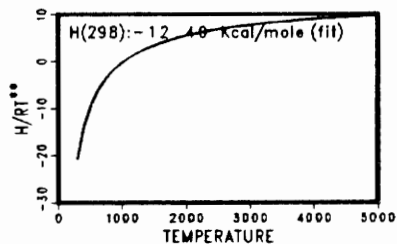
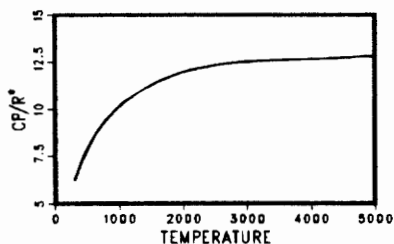
KETENE

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02974970E+02 | 0.12118712E-01 | -0.02345045E-04 | -0.06466685E-07 | 0.03905649E-10  | -0.07632636E+05 | 0.08673553E+02  |
| 1000-5000K   | 0.06038817E+02 | 0.05804840E-01 | -0.01920953E-04 | 0.02794484E-08  | -0.14588676E-13 | -0.08563402E+05 | -0.07657581E+02 |

Source: BURCAT (C<sub>2</sub>H<sub>2</sub>O) (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>2</sub>F<sub>2</sub>

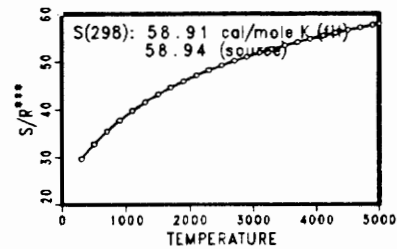
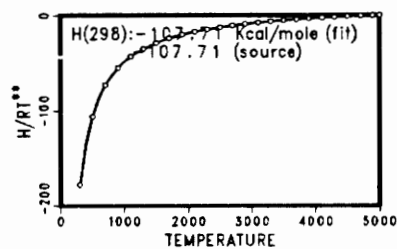
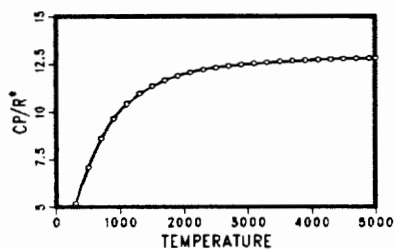
DIFLUOROMETHANE

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.03669433E+01 | 0.02168917E+00 | -0.02441912E-03 | 0.01942310E-06 | -0.06978343E-10 | -0.05510102E+06 | 0.02202214E+03  |
| 1000-5000K   | 0.04730052E+02 | 0.07997300E-01 | -0.03186045E-04 | 0.05801159E-08 | -0.03967925E-12 | -0.05637288E+06 | -0.04954843E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

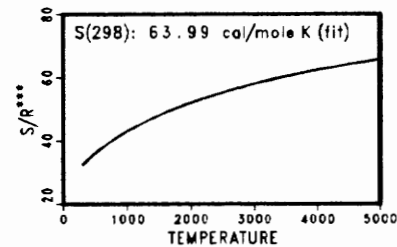
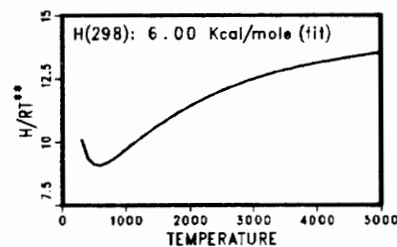
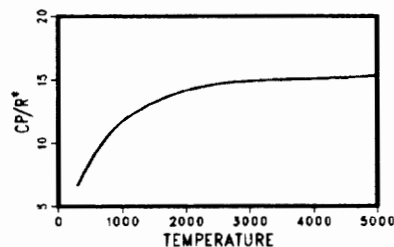
Species: CH<sub>2</sub>HCOCH<sub>2</sub>HCO RAD

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03409062E+02 | 0.10738574E-01 | 0.01891492E-04  | -0.07158583E-07 | 0.02867385E-10  | 0.15214766E+04 | 0.09558290E+02  |
| 1000-5000K   | 0.05975670E+02 | 0.08130591E-01 | -0.02743624E-04 | 0.04070304E-08  | -0.02176017E-12 | 0.04903218E+04 | -0.05045251E+02 |

Source: BURCAT, C<sub>2</sub>H<sub>3</sub>OA (CH<sub>2</sub>CHO) (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH2O

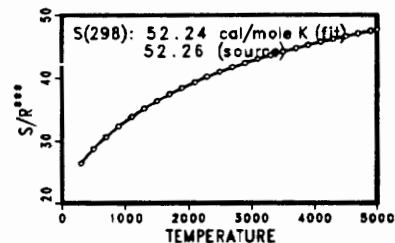
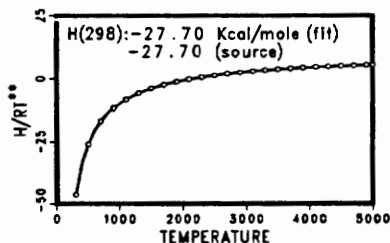
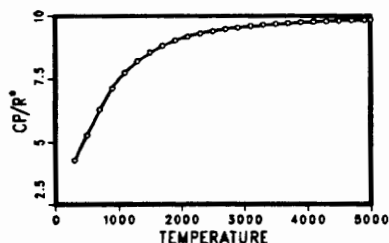
FORMALDEHYDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.16527311E+01 | 0.12631439E-01 | -0.01888168E-03 | 0.02050031E-06 | -0.08413237E-10 | -0.14865404E+05 | 0.13784820E+02 |
| 1000-5000K   | 0.02995606E+02 | 0.06681321E-01 | -0.02628954E-04 | 0.04737153E-08 | -0.03212517E-12 | -0.15320369E+05 | 0.06912572E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned}
 * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: CH2OH

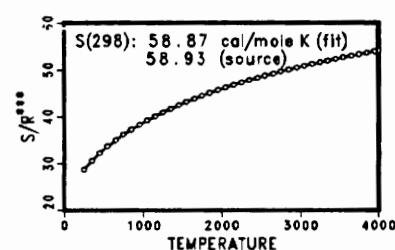
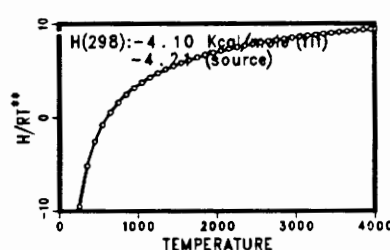
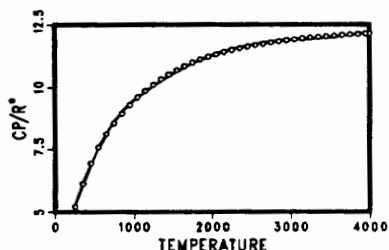
HYDROXYMETHYLENE RAD

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0250-1000K   | 0.02862628E+02 | 0.10015273E-01 | -0.05285435E-05 | -0.05138539E-07 | 0.02246041E-10 | -0.03349678E+05 | 0.10397938E+02  |
| 1000-4000K   | 0.06327520E+02 | 0.03608270E-01 | -0.03201547E-05 | -0.01938750E-08 | 0.03509704E-12 | -0.04474509E+05 | -0.08329365E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: CH3

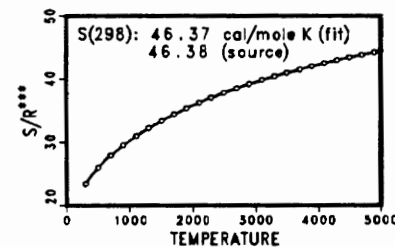
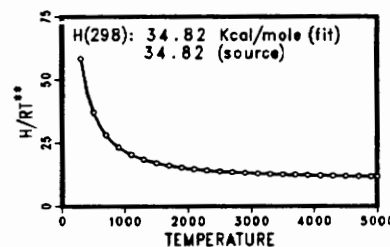
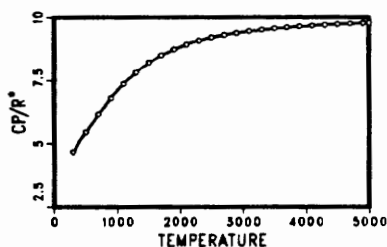
METHYL

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02430442E+02 | 0.11124099E-01 | -0.01680220E-03 | 0.16218288E-07 | -0.05864952E-10 | 0.16423781E+05 | 0.06789794E+02 |
| 1000-5000K   | 0.02844051E+02 | 0.06137974E-01 | -0.02230345E-04 | 0.03785161E-08 | -0.02452159E-12 | 0.16437809E+05 | 0.05452697E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned}
 * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: CH3CC

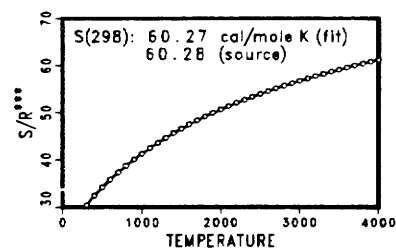
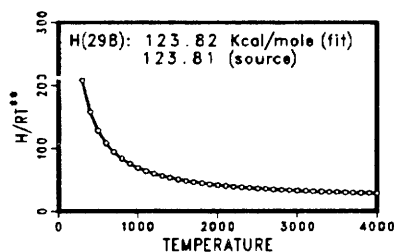
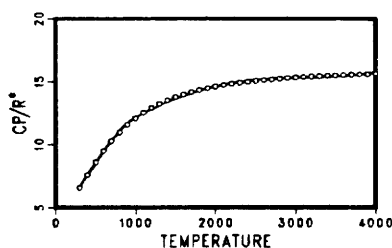
1-PROPYNYL C3V 2A1

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03798751E+02 | 0.08749062E-01 | 0.02523014E-04  | -0.15293730E-08 | -0.14105619E-11 | 0.06077425E+06 | 0.05989223E+02  |
| 1000-4000K   | 0.07640221E+02 | 0.05233556E-01 | -0.05053635E-05 | -0.02919772E-08 | 0.05445700E-12  | 0.05909763E+06 | -0.16295735E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH3CCCH2

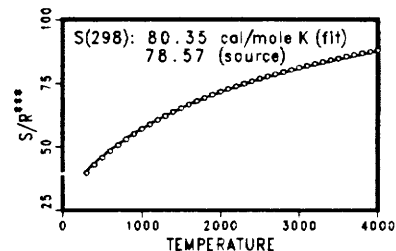
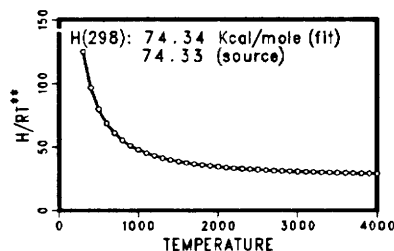
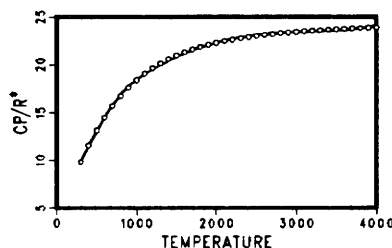
HCCC CIS

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.05068450E+02 | 0.15717475E-01 | 0.02968975E-04  | -0.04990586E-07 | -0.02984224E-11 | 0.03518855E+06 | 0.06791893E+02  |
| 1000-4000K   | 0.11565059E+02 | 0.08030297E-01 | -0.07649450E-05 | -0.04476533E-08 | 0.08313260E-12  | 0.03256813E+06 | -0.03014066E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH3CCCH3

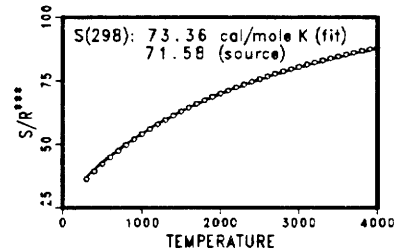
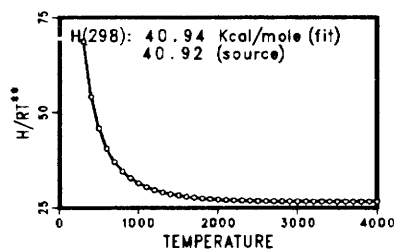
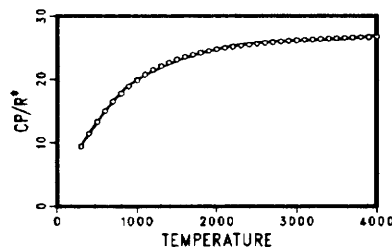
2-BUTYNE

GAS

As of: 12/01/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04077105E+02 | 0.01703158E+00 | 0.04707490E-04  | -0.03767239E-07 | -0.02066962E-10 | 0.01859756E+06 | 0.08444801E+02  |
| 1000-4000K   | 0.11336582E+02 | 0.10057637E-01 | -0.09511323E-05 | -0.05660496E-08 | 0.10494509E-12  | 0.15476594E+05 | -0.03350866E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>3</sub>CCH<sub>2</sub>

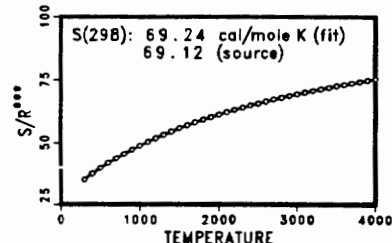
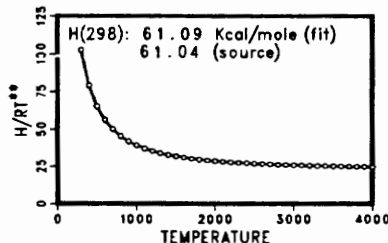
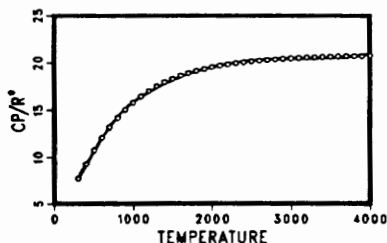
1-METHYL-ETHENYL CS 2A'

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.0338581E+02  | 0.14045337E-01 | 0.03204127E-04  | -0.03824120E-07 | -0.09053742E-11 | 0.02909066E+06 | 0.11266487E+02  |
| 1000-4000K   | 0.09101018E+02 | 0.07964167E-01 | -0.07884945E-05 | -0.04562036E-08 | 0.08529212E-12  | 0.02670680E+06 | -0.02150559E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>3</sub>CH<sub>2</sub>CCH

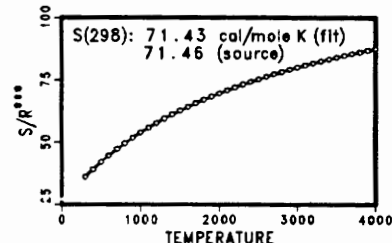
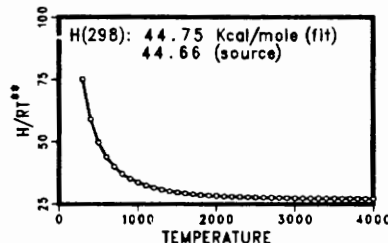
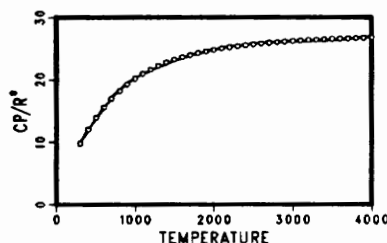
1-BUTYNE

GAS

As of: 12/01/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03726043E+02 | 0.02053492E+00 | 0.03021439E-04  | -0.08131812E-07 | 0.10952799E-11 | 0.02048821E+06 | 0.08538826E+02  |
| 1000-4000K   | 0.12006946E+02 | 0.09576069E-01 | -0.08995018E-05 | -0.05369808E-08 | 0.09934174E-12 | 0.01729419E+06 | -0.03802692E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>3</sub>CHCH

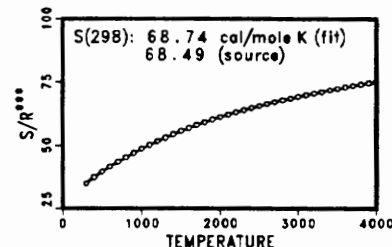
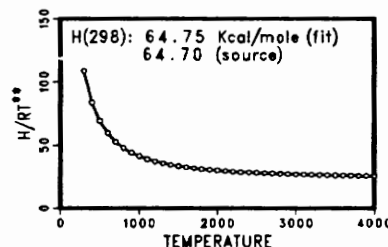
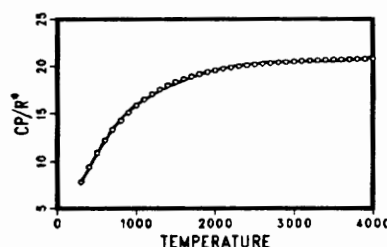
PROP-1-ENYL HC=CHCIS 2A'

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03161863E+02 | 0.15180997E-01 | 0.02722659E-04  | -0.05177112E-07 | 0.05435286E-12 | 0.03095547E+06 | 0.11979733E+02  |
| 1000-4000K   | 0.09209764E+02 | 0.07871412E-01 | -0.07724522E-05 | -0.04497357E-08 | 0.08377272E-12 | 0.02853967E+06 | -0.02232369E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH3CL

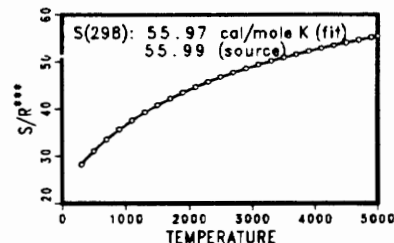
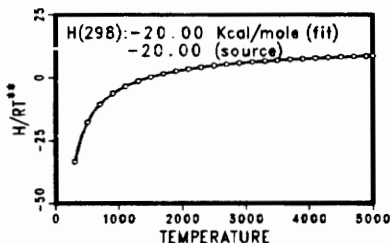
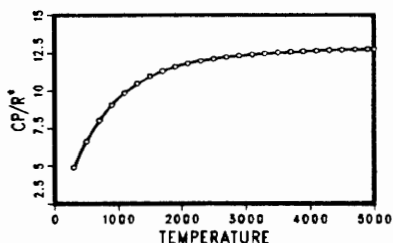
METHYL CHLORIDE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.04621901E+01 | 0.02068247E+00 | -0.02553133E-03 | 0.02160310E-06 | -0.07706816E-10 | -0.10936672E+05 | 0.02032976E+03 |
| 1000-5000K   | 0.03633875E+02 | 0.08664625E-01 | -0.03343871E-04 | 0.05950130E-08 | -0.04001401E-12 | -0.11776588E+05 | 0.04430651E+02 |



Source: SNLL FIT TO JANNAF DATA

Comments: ALSO CALLED CHLOROMETHANE

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH3CO

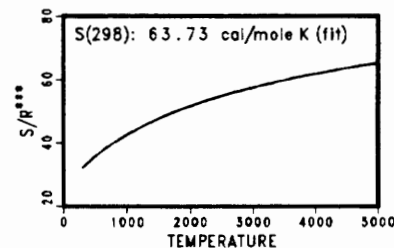
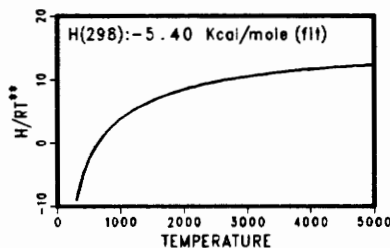
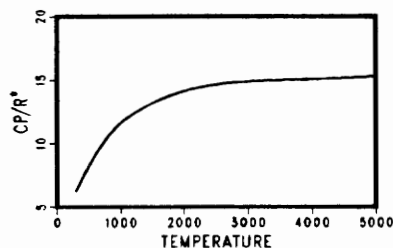
CH3CO RAD

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.03125278E+02 | 0.09778220E-01 | 0.04521448E-04  | -0.09009462E-07 | 0.03193717E-10  | -0.04108507E+05 | 0.11228854E+02  |
| 1000-5000K   | 0.05612279E+02 | 0.08449886E-01 | -0.02854147E-04 | 0.04238376E-08  | -0.02268403E-12 | -0.05187863E+05 | -0.03274949E+02 |



Source: BURCAT C2H3OB (CH3CO) (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH3F

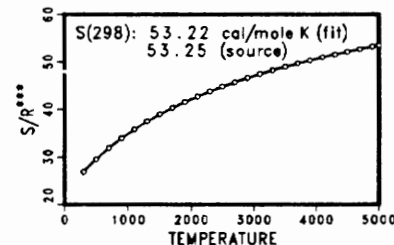
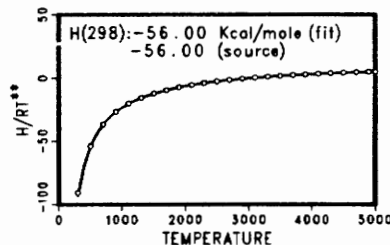
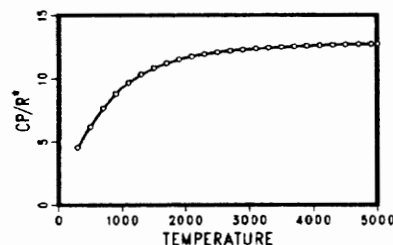
FLUOROMETHANE

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.02600910E+01 | 0.02000787E+00 | -0.02662584E-03 | 0.02561176E-06 | -0.09935237E-10 | -0.02896232E+06 | 0.02031799E+03 |
| 1000-5000K   | 0.03014978E+02 | 0.09314397E-01 | -0.03611697E-04 | 0.06443728E-08 | -0.04339594E-12 | -0.02977838E+06 | 0.06323815E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>3</sub>HCO

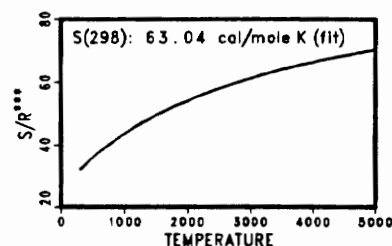
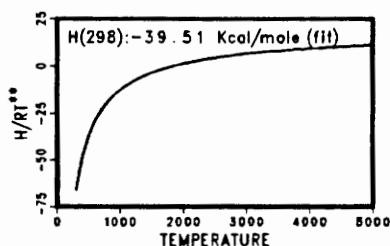
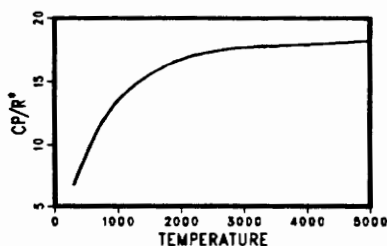
ACETALDEHYDE

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02505695E+02 | 0.13369907E-01 | 0.04671953E-04  | -0.11281401E-07 | 0.04263566E-10  | -0.02124588E+06 | 0.13350887E+02  |
| 1000-5000K   | 0.05868650E+02 | 0.10794241E-01 | -0.03645530E-04 | 0.05412912E-08  | -0.02896844E-12 | -0.02264568E+06 | -0.06012946E+02 |



Source: BURCAT (C2H40A) (TECHNION REPORTS)

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: CH<sub>3</sub>O

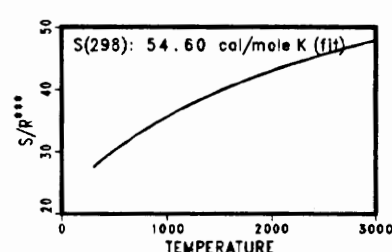
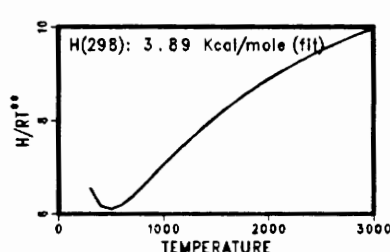
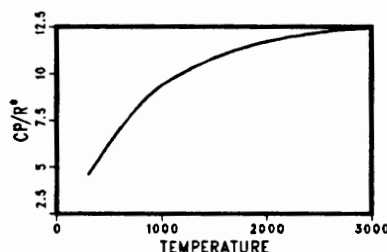
METHYLOXIDE (METHOXY RAD)

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02106204E+02 | 0.07216595E-01 | 0.05338472E-04  | -0.07377636E-07 | 0.02075610E-10  | 0.09786011E+04 | 0.13152177E+02 |
| 1000-3000K   | 0.03770799E+02 | 0.07871497E-01 | -0.02656384E-04 | 0.03944431E-08  | -0.02112616E-12 | 0.12783252E+03 | 0.02929575E+02 |



Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: CH<sub>3</sub>OH

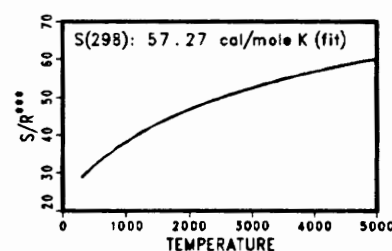
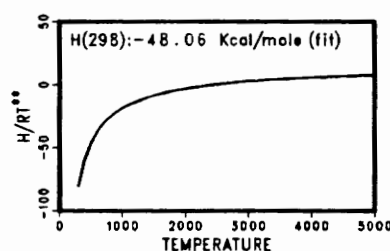
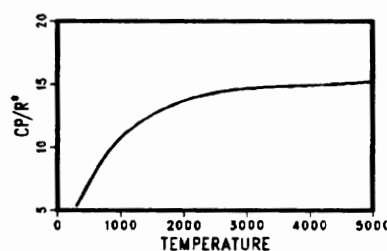
METHANOL

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.02660115E+02 | 0.07341508E-01 | 0.07170050E-04  | -0.08793194E-07 | 0.02390570E-10  | -0.02535348E+06 | 0.11232631E+02 |
| 1000-5000K   | 0.04029061E+02 | 0.09376593E-01 | -0.03050254E-04 | 0.04358793E-08  | -0.02224723E-12 | -0.02615791E+06 | 0.02378195E+02 |



Source: BURCAT (CH40) (TECHNION REPORTS)

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$



Species: CH<sub>3</sub>SICL<sub>3</sub>

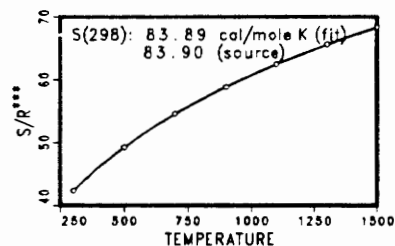
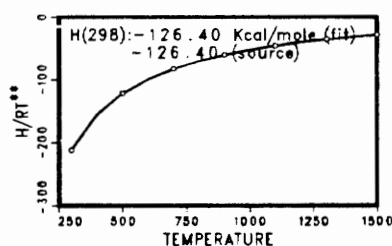
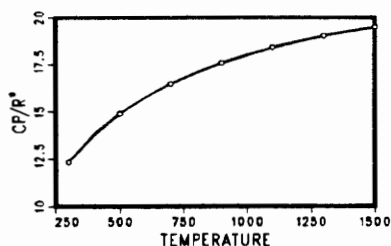
TRICHLOROMETHYLSILANE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.04637712E+02 | 0.03733016E+00 | -0.04798528E-03 | 0.03353132E-06  | -0.09484405E-10 | -0.06629348E+06 | 0.06524867E+02  |
| 1000-1500K   | 0.11803988E+02 | 0.07642902E-01 | -0.09493348E-06 | -0.01852654E-07 | 0.05302190E-11  | -0.06773651E+06 | -0.02794492E+03 |



Source: SNLL FIT TO JANNAF DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>4</sub>

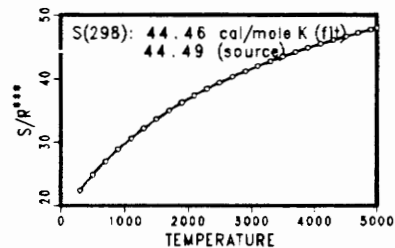
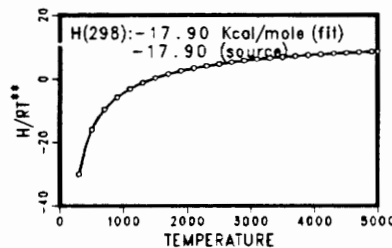
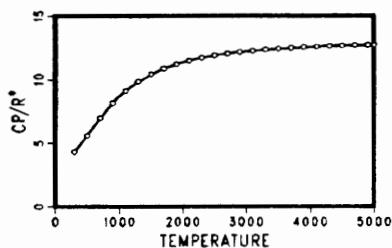
METHANE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.07787415E+01 | 0.01747668E+00 | -0.02783409E-03 | 0.03049708E-06 | -0.12239307E-10 | -0.09825229E+05 | 0.13722195E+02 |
| 1000-5000K   | 0.01683478E+02 | 0.10237236E-01 | -0.03875128E-04 | 0.06785585E-08 | -0.04503423E-12 | -0.10080787E+05 | 0.09623395E+02 |



Source: SNLL FIT TO JANNAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CHCL

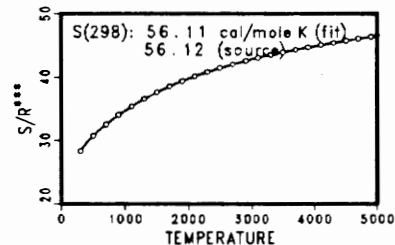
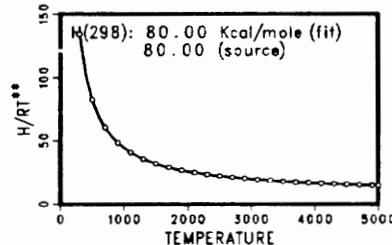
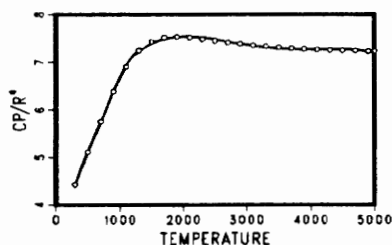
MONOCHLOROMETHYLENE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1200K   | 0.02781262E+02 | 0.07805384E-01 | -0.10637111E-04 | 0.10654407E-07 | -0.03916796E-10 | 0.03916144E+06 | 0.10455153E+02 |
| 1200-5000K   | 0.03216518E+02 | 0.05976969E-01 | -0.02918238E-04 | 0.05912801E-08 | -0.04297945E-12 | 0.03879839E+06 | 0.07793842E+02 |



Source: SNLL FIT TO JANNAF DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CHCL3

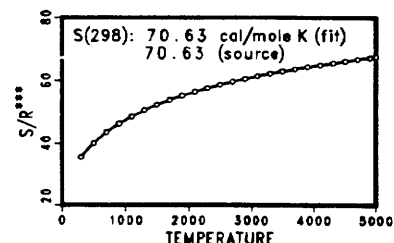
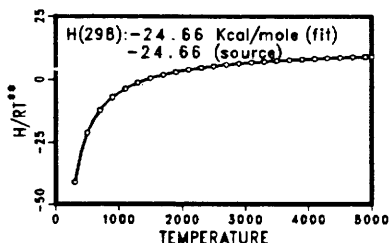
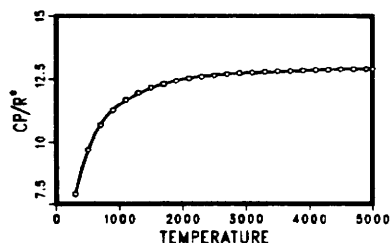
CHLOROFORM

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.03437633E+02 | 0.01941496E+00 | -0.16494730E-04 | 0.05196545E-07 | -0.06939614E-12 | -0.14161262E+05 | 0.10863299E+02  |
| 1000-5000K   | 0.08523544E+02 | 0.04480142E-01 | -0.01837282E-04 | 0.03424891E-08 | -0.02387283E-12 | -0.15461167E+05 | -0.15056193E+02 |



Source: SNLL FIT TO JANNAF DATA  
Comments: ALSO CALLED TRICHLOROMETHANE

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CHF

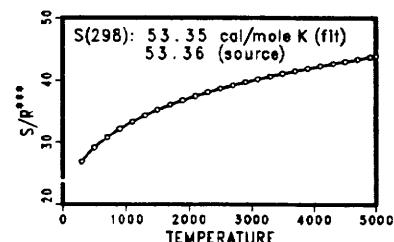
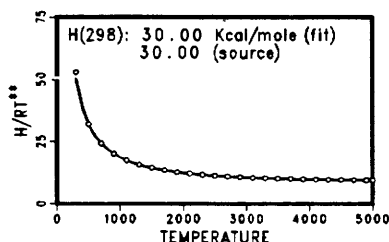
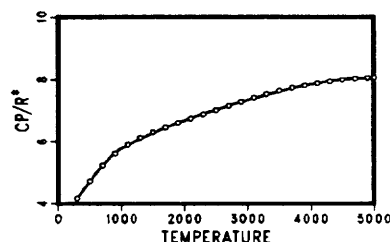
MONOFLUOROMETHYLENE

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03029060E+02 | 0.04850873E-01 | -0.04971678E-04 | 0.05277968E-07 | -0.02403154E-10 | 0.14014348E+05 | 0.08324101E+02 |
| 1000-5000K   | 0.04242812E+02 | 0.02066316E-01 | -0.06527951E-05 | 0.13887000E-09 | -0.12133360E-13 | 0.13559817E+05 | 0.01680196E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CHF3

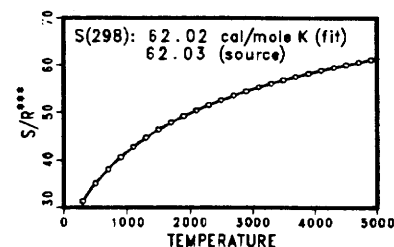
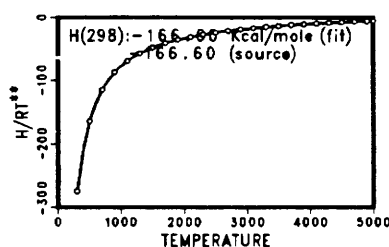
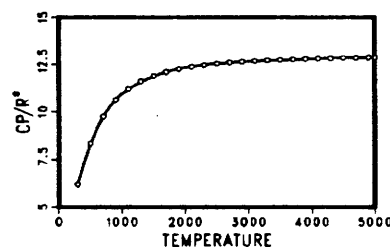
TRIFLUOROMETHANE

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.08725142E+01 | 0.02308431E+00 | -0.02123718E-03 | 0.11144284E-07 | -0.02909229E-10 | -0.08496391E+06 | 0.02021498E+03  |
| 1000-5000K   | 0.06834333E+02 | 0.06248730E-01 | -0.02575750E-04 | 0.04809112E-08 | -0.03352074E-12 | -0.08663771E+06 | -0.10627405E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CL

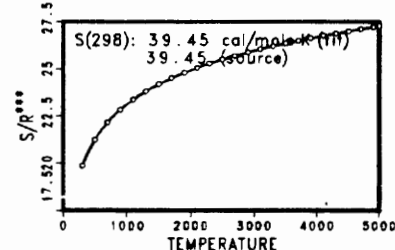
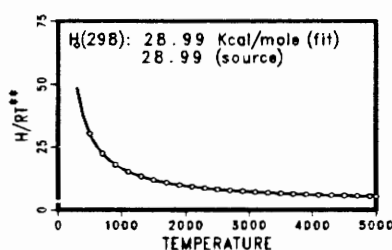
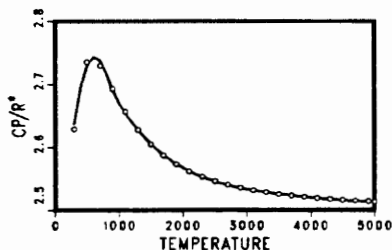
CHLORINE, MONATOMIC

GAS

As of: 4/21/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.02381576E+02 | 0.08891079E-02  | 0.04070475E-05 | -0.02168943E-07 | 0.11608274E-11 | 0.13839987E+05 | 0.06021817E+02 |
| 1000-5000K   | 0.02920235E+02 | -0.03597985E-02 | 0.12942943E-06 | -0.02162776E-09 | 0.13765171E-14 | 0.13713381E+05 | 0.03262690E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CL2

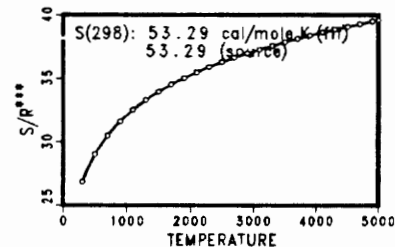
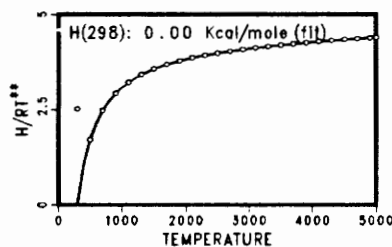
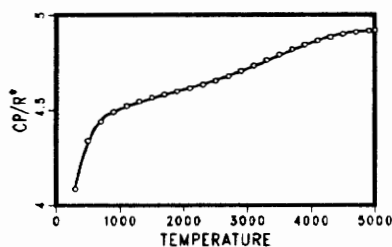
CHLORINE, DIATOMIC

GAS

As of: 4/21/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03439587E+02 | 0.02870774E-01 | -0.02385870E-04 | 0.02892918E-08 | 0.02915057E-11  | -0.11317875E+04 | 0.06471359E+02 |
| 1000-5000K   | 0.04274586E+02 | 0.03717336E-02 | -0.01893489E-05 | 0.05337465E-09 | -0.05057602E-13 | -0.13311486E+04 | 0.02256946E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CN

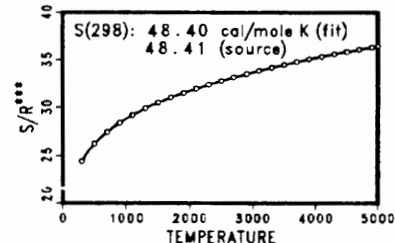
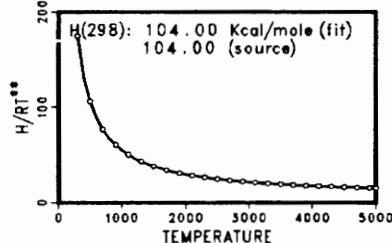
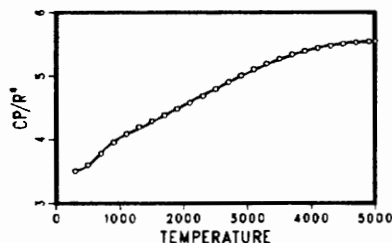
CYANO

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03663204E+02 | -0.11565290E-02 | 0.02163409E-04 | 0.01854208E-08  | -0.08214695E-11 | 0.05128118E+06 | 0.03739015E+02 |
| 1000-5000K   | 0.03720119E+02 | 0.15183506E-03  | 0.01987381E-05 | -0.03798371E-09 | 0.13282296E-14  | 0.05111626E+06 | 0.02888597E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CN+

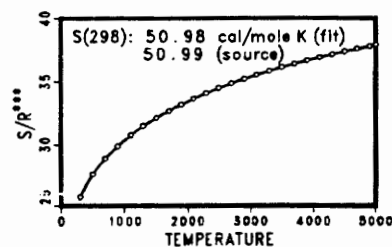
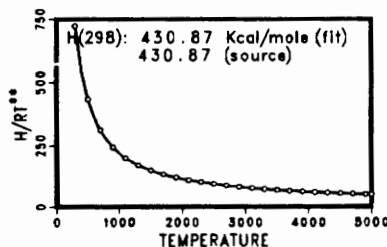
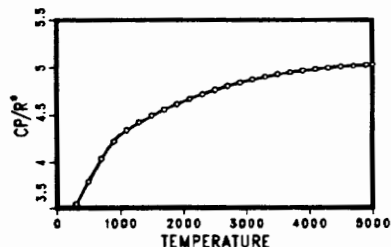
CYANO, UNIPosITIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03118657E+02 | 0.15532581E-02 | -0.09487764E-05 | 0.14795005E-08 | -0.09096763E-11 | 0.02158512E+07 | 0.07456254E+02 |
| 1000-5000K   | 0.03701463E+02 | 0.07482931E-02 | -0.01790173E-05 | 0.02366368E-09 | -0.14370368E-14 | 0.02155966E+07 | 0.04108678E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CN-

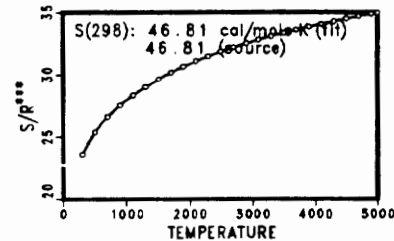
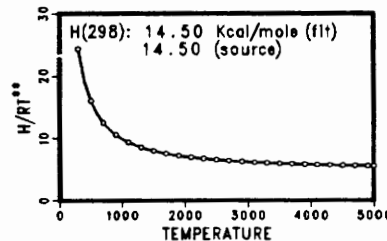
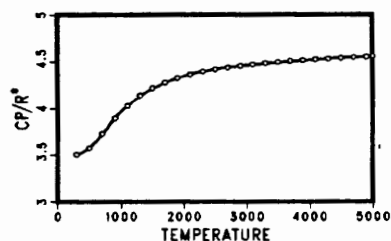
CYANO, UNINEGATIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03278995E+02 | 0.14641916E-02 | -0.03925899E-04 | 0.05629874E-07 | -0.02473496E-10 | 0.06279509E+05 | 0.04568972E+02 |
| 1000-5000K   | 0.02981276E+02 | 0.14647728E-02 | -0.05672737E-05 | 0.10176226E-09 | -0.06870930E-13 | 0.06346098E+05 | 0.06171693E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CN2

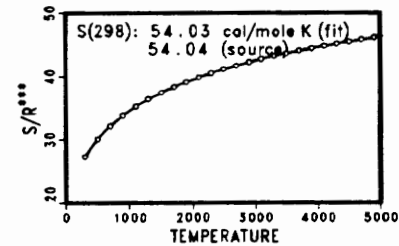
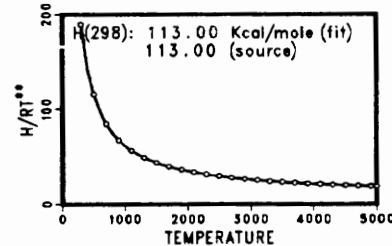
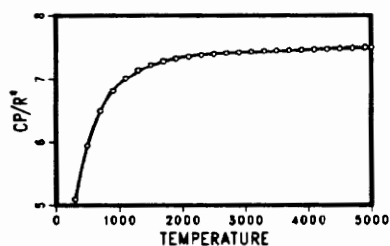
NCN RADICAL

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03039963E+02 | 0.08812105E-01 | -0.07605508E-04 | 0.03554357E-07 | -0.08746100E-11 | 0.05563268E+06 | 0.07555298E+02  |
| 1000-5000K   | 0.05567064E+02 | 0.02100501E-01 | -0.09010517E-05 | 0.01718571E-08 | -0.12062552E-13 | 0.05489968E+06 | -0.05630054E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CNN

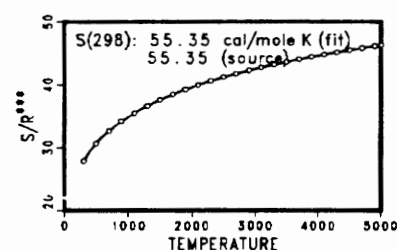
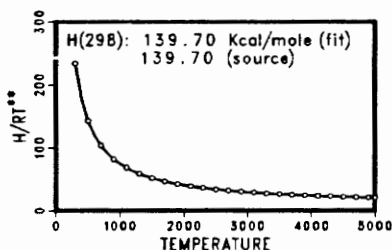
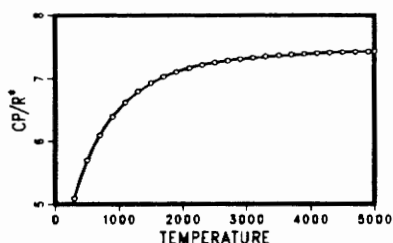
CNN RADICAL

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03524436E+02 | 0.07271923E-01 | -0.08272698E-04 | 0.05628704E-07 | -0.16415759E-11 | 0.06899647E+06 | 0.05932444E+02  |
| 1000-5000K   | 0.04785930E+02 | 0.02559553E-01 | -0.10031326E-05 | 0.01807148E-08 | -0.12273827E-13 | 0.06870411E+06 | -0.02953957E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CO

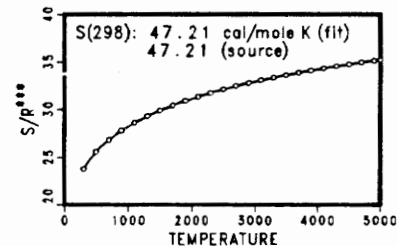
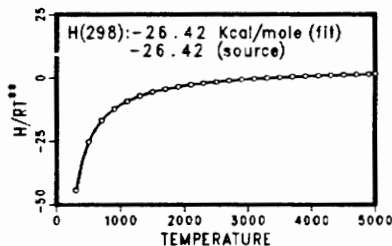
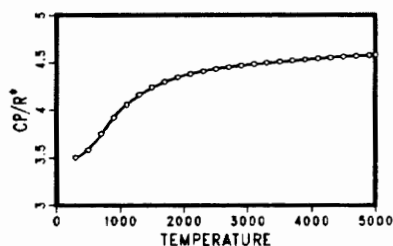
CARBON MONOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03262451E+02 | 0.15119409E-02 | -0.03881755E-04 | 0.05581944E-07 | -0.02474951E-10 | -0.14310539E+05 | 0.04848897E+02 |
| 1000-5000K   | 0.03025078E+02 | 0.14426885E-02 | -0.05630827E-05 | 0.10185813E-09 | -0.06910951E-13 | -0.14268350E+05 | 0.06108217E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CO2

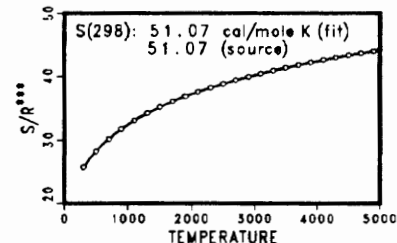
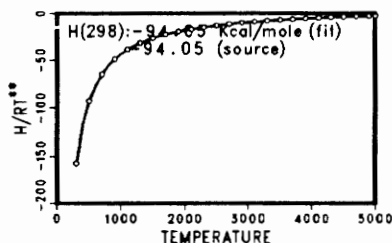
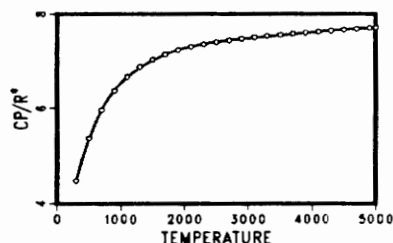
CARBON DIOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02275724E+02 | 0.09922072E-01 | -0.10409113E-04 | 0.06866686E-07 | -0.02117280E-10 | -0.04837314E+06 | 0.10188488E+02  |
| 1000-5000K   | 0.04453623E+02 | 0.03140168E-01 | -0.12784105E-05 | 0.02393996E-08 | -0.16690333E-13 | -0.04896696E+06 | -0.09553959E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CO2-

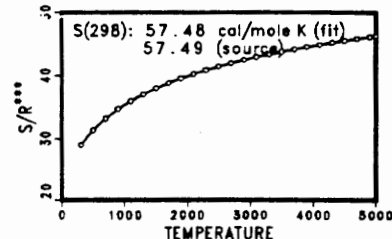
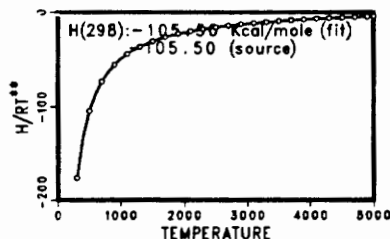
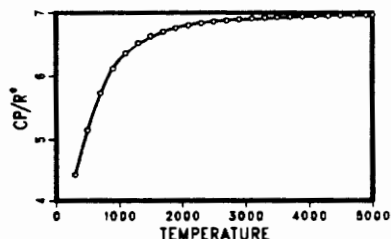
CARBON DIOXIDE, UNINEGATIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.02637077E+02 | 0.07803230E-01 | -0.08196187E-04 | 0.06537897E-07 | -0.02520220E-10 | -0.05416772E+06 | 0.11889549E+02 |
| 1000-5000K   | 0.04610574E+02 | 0.02532962E-01 | -0.10701653E-05 | 0.02026770E-08 | -0.14249581E-13 | -0.05479881E+06 | 0.14496295E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: COS

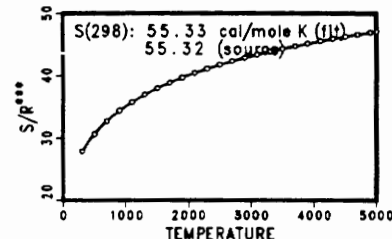
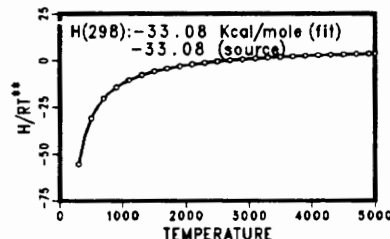
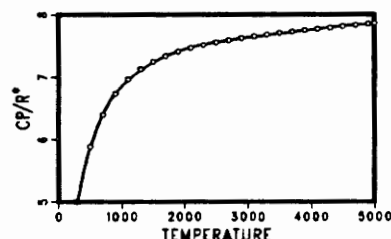
CARBON OXYSULFIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02858530E+02 | 0.09515458E-01 | -0.08884915E-04 | 0.04220994E-07 | -0.08557340E-11 | -0.01785144E+06 | 0.09081989E+02  |
| 1000-5000K   | 0.05191924E+02 | 0.02506123E-01 | -0.10243963E-05 | 0.01943914E-08 | -0.13707999E-13 | -0.01846210E+06 | -0.02825755E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CS

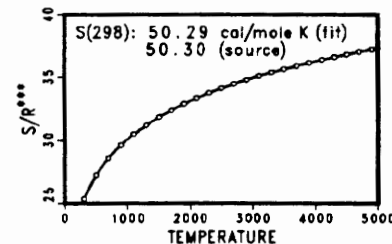
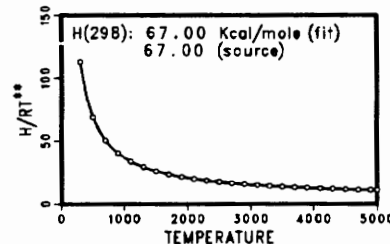
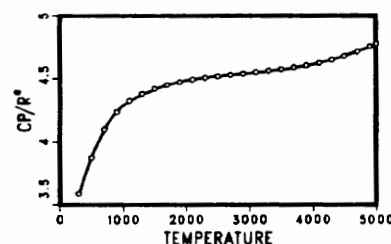
CARBON MONOSULFIDE

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02938623E+02 | 0.02724351E-01 | -0.02397706E-04 | 0.01689500E-07 | -0.06665050E-11 | 0.03273992E+06 | 0.07848720E+02 |
| 1000-5000K   | 0.03737430E+02 | 0.08180451E-02 | -0.03178918E-05 | 0.05356801E-09 | -0.02886194E-13 | 0.03247725E+06 | 0.03576556E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CS2

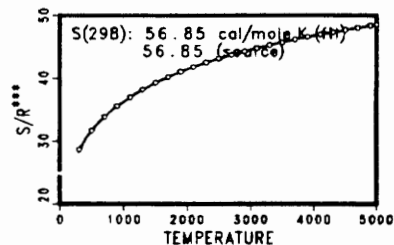
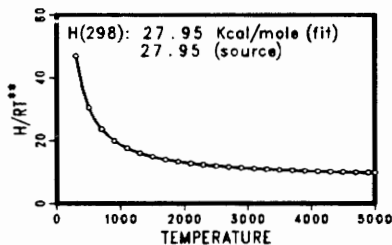
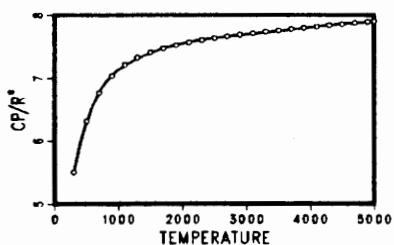
CARBON DISULFIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03566139E+02 | 0.08374927E-01 | -0.06835704E-04 | 0.02091214E-07 | -0.06737193E-12 | 0.12688482E+05 | 0.06085967E+02  |
| 1000-5000K   | 0.05930515E+02 | 0.01813645E-01 | -0.07492172E-05 | 0.14458920E-09 | -0.10326380E-13 | 0.12051166E+05 | -0.06093909E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: E

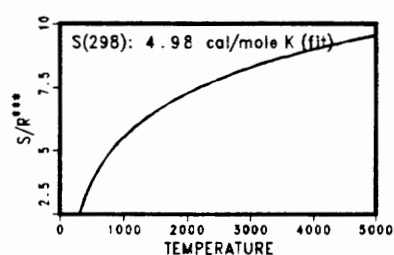
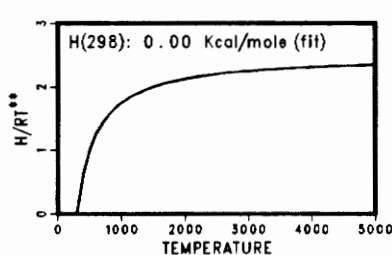
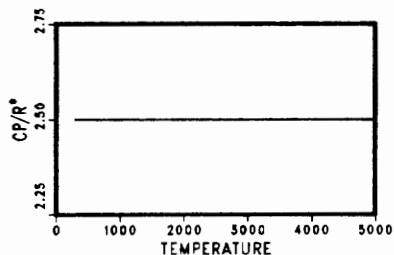
ELECTRON

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | -0.07453750E+04 | -0.11734026E+02 |
| 1000-5000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | -0.07453749E+04 | -0.11734026E+02 |



Source: NASA FIT TO NASA-LEWIS DATA

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: F

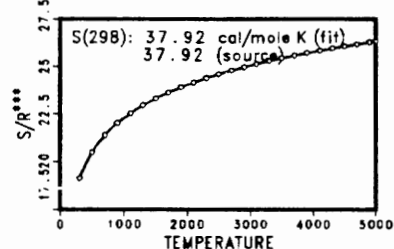
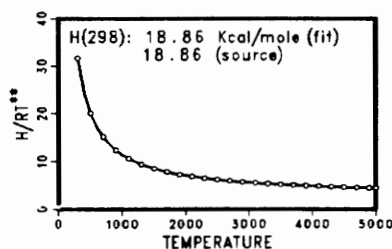
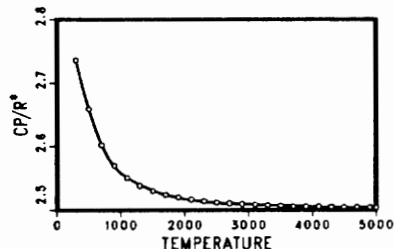
FLUORINE, MONATOMIC

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.02913904E+02 | -0.07336339E-02 | 0.05571015E-05 | -0.02666871E-08 | 0.08643255E-12 | 0.08651201E+05 | 0.02677115E+02 |
| 1000-5000K   | 0.02687459E+02 | -0.02010358E-02 | 0.08597957E-06 | -0.16449738E-10 | 0.11661605E-14 | 0.08722883E+05 | 0.03882212E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: F2

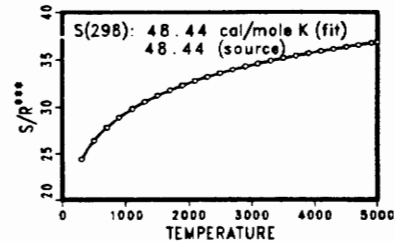
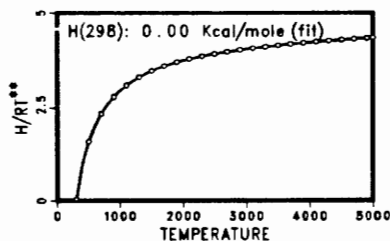
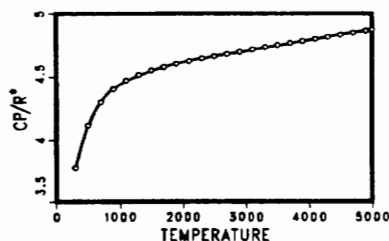
FLUORINE, DIATOMIC (REF ST)

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.02940287E+02 | 0.03491491E-01 | -0.02458207E-04 | 0.01837073E-08 | 0.02850916E-11  | -0.10104296E+04 | 0.06694194E+02 |
| 1000-5000K   | 0.04018308E+02 | 0.06221479E-02 | -0.02420845E-05 | 0.04742076E-09 | -0.03418141E-13 | -0.13007128E+04 | 0.11263273E+01 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

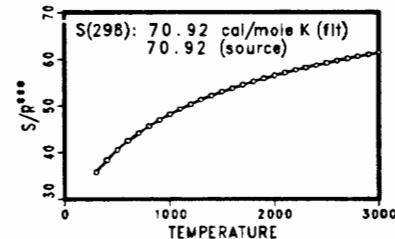
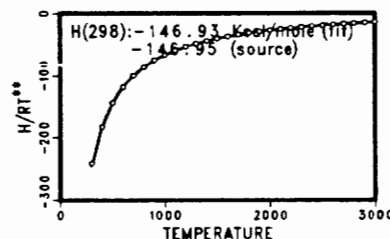
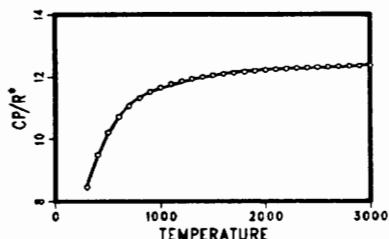
Species: F2SINH

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.04951547E+02 | 0.13296361E-01 | -0.02098648E-04 | -0.10072757E-07 | 0.05552285E-10 | -0.07597540E+06 | 0.03690891E+02  |
| 1000-3000K   | 0.10048301E+02 | 0.01983144E-01 | -0.02703168E-05 | -0.01767852E-08 | 0.04444367E-12 | -0.07739741E+06 | -0.02303888E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: F3SIN

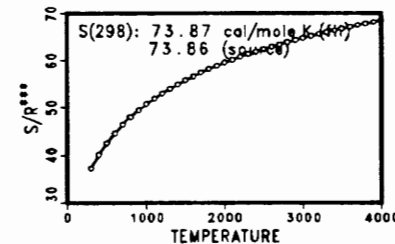
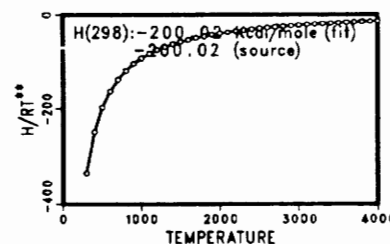
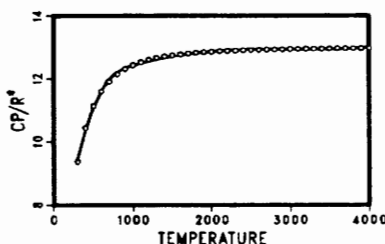
TRIFLUOROSILYLNITRENE

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.06028419E+02 | 0.12786807E-01 | -0.01878856E-04 | -0.09695426E-07 | 0.05184847E-10 | -0.10299499E+06 | -0.08217830E+01 |
| 1000-4000K   | 0.11512423E+02 | 0.11150295E-02 | -0.16054655E-06 | -0.05271933E-09 | 0.11608998E-13 | -0.10459191E+06 | -0.02981224E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$



Species: FNNF

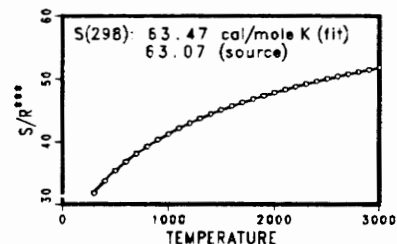
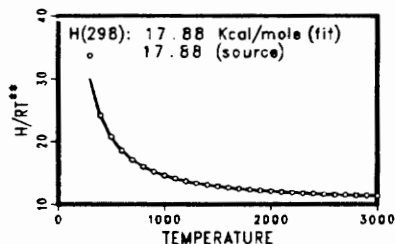
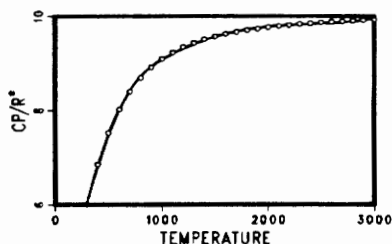
CIS-DIFLUORODIAZINE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03127143E+02 | 0.10571342E-01 | -0.09746113E-05 | -0.07208357E-07 | 0.03567978E-10 | 0.07615830E+05 | 0.11074648E+02  |
| 1000-3000K   | 0.07255211E+02 | 0.02274409E-01 | -0.02793346E-05 | -0.02203843E-08 | 0.05359234E-12 | 0.06360352E+05 | -0.10942477E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: FN03

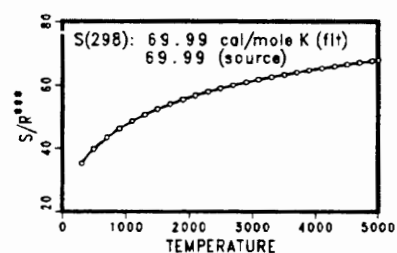
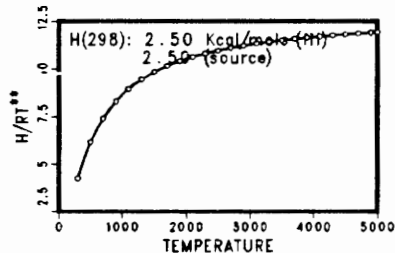
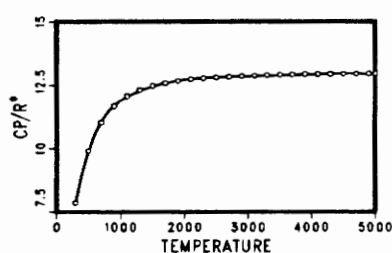
FLUORINE NITRATE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02985786E+02 | 0.02094642E+00 | -0.16527329E-04 | 0.04318770E-07 | 0.16607836E-12  | -0.04237215E+04 | 0.12667929E+02  |
| 1000-5000K   | 0.09176275E+02 | 0.04219072E-01 | -0.01835575E-04 | 0.03553717E-08 | -0.02541078E-12 | -0.02118638E+05 | -0.01934397E+03 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: FO

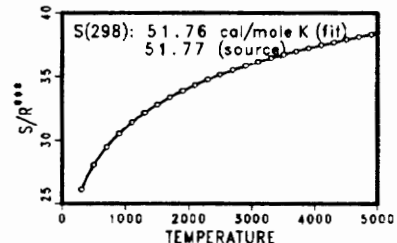
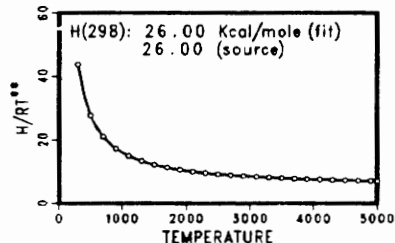
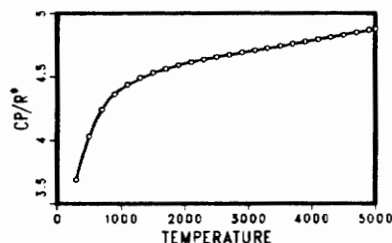
FLUORINE MONOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02879578E+02 | 0.03399121E-01 | -0.02572854E-04 | 0.07422381E-08 | -0.04328053E-12 | 0.12096633E+05 | 0.08738887E+02 |
| 1000-5000K   | 0.03913735E+02 | 0.07210714E-02 | -0.02796614E-05 | 0.05337821E-09 | -0.03720183E-13 | 0.11801406E+05 | 0.03346367E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: F02

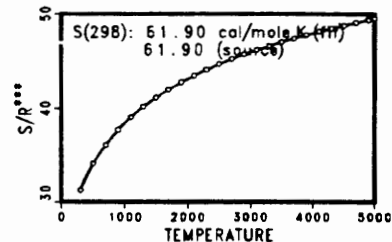
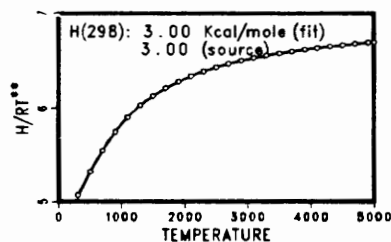
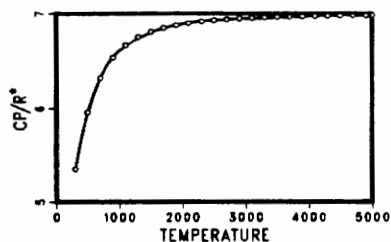
DIOXYGEN FLUORIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.03872542E+02 | 0.06409974E-01 | -0.05517784E-04 | 0.02232770E-07 | -0.03876157E-11 | 0.11570760E+03  | 0.07406949E+02  |
| 1000-5000K   | 0.05678971E+02 | 0.14424551E-02 | -0.06229546E-05 | 0.11996118E-09 | -0.08543416E-13 | -0.03861836E+04 | -0.01941811E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned}
 \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 \bullet\bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 \bullet\bullet\bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

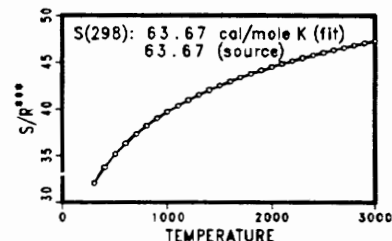
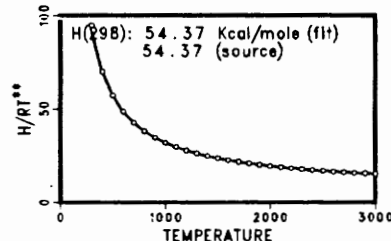
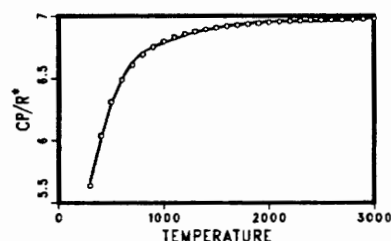
Species: FSIN

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.04269969E+02 | 0.05298358E-01 | -0.11038015E-05 | -0.03962805E-07 | 0.02282982E-10 | 0.02587238E+06 | 0.06215038E+02  |
| 1000-3000K   | 0.06269572E+02 | 0.06747867E-02 | -0.12419759E-06 | -0.04970158E-09 | 0.14244521E-13 | 0.02533350E+06 | -0.04201141E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 \bullet\bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 \bullet\bullet\bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

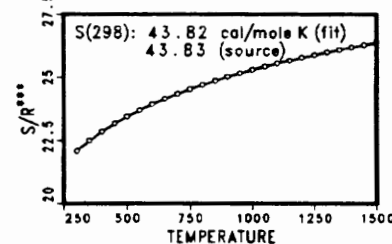
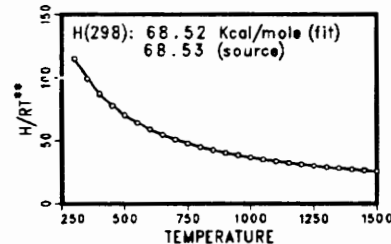
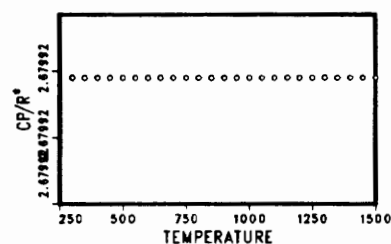
Species: GA

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.02679919E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.03368803E+06 | 0.06788109E+02 |
| 0600-1500K   | 0.02679919E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.03368804E+06 | 0.06788109E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned}
 \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 \bullet\bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 \bullet\bullet\bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

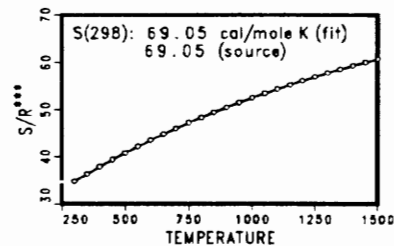
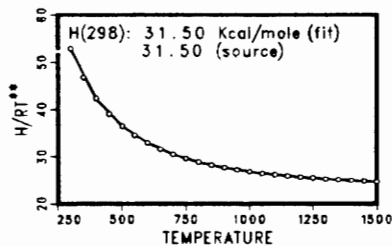
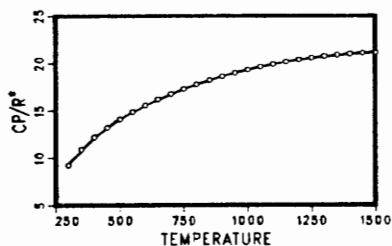
Species: GA2H6

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | -0.03914560E+02 | 0.04965434E+00 | 0.07401903E-04  | -0.11241373E-06 | 0.08726339E-09 | 0.14930795E+05 | 0.04274882E+03  |
| 0600-1500K   | 0.06016247E+02  | 0.01788370E+00 | -0.12042288E-06 | -0.06487881E-07 | 0.02075367E-10 | 0.13125479E+05 | -0.05228029E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

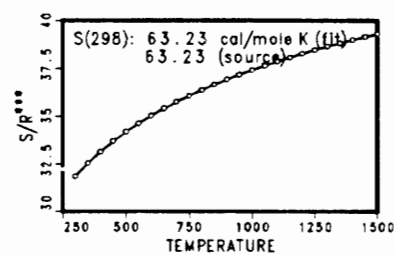
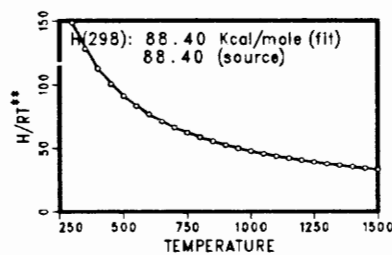
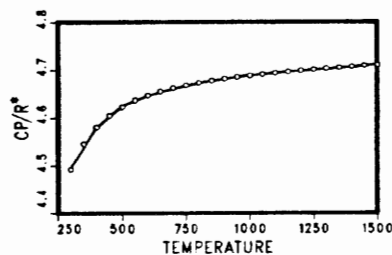
Species: GAAS

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.03967473E+02 | 0.02318966E-01 | -0.1454521E-05  | -0.03411430E-07 | 0.03365821E-10 | 0.04321919E+06 | 0.08599628E+02 |
| 0600-1500K   | 0.04471149E+02 | 0.04238449E-02 | -0.02279404E-05 | -0.04441172E-10 | 0.02618952E-12 | 0.04313359E+06 | 0.06212470E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

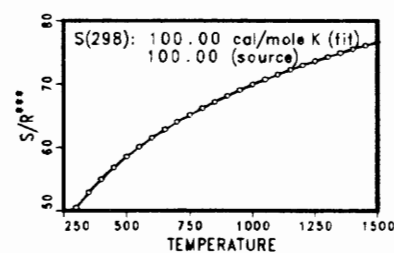
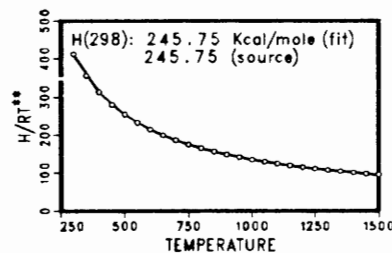
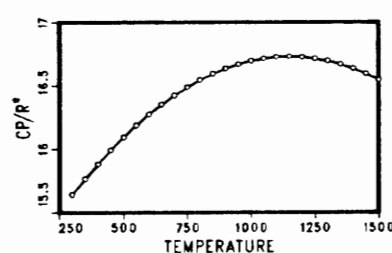
Species: GAAS(3,C)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-0600K   | 0.14701892E+02 | 0.03827728E-01 | -0.02945747E-04 | 0.02465370E-07  | -0.15205979E-11 | 0.11914958E+06 | -0.03445955E+03 |
| 0600-1500K   | 0.14852467E+02 | 0.02959435E-01 | -0.07124246E-05 | -0.05316048E-08 | 0.12873211E-12  | 0.11912617E+06 | -0.03514144E+03 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

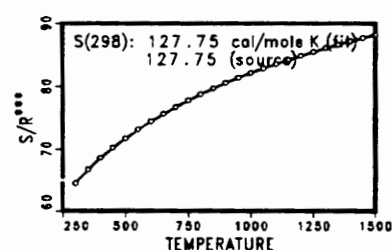
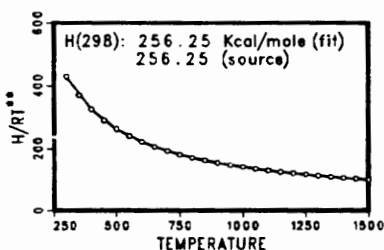
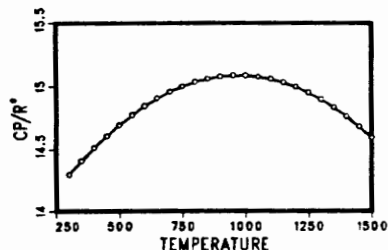
Species: GAAS(3,L)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-0600K   | 0.13412763E+02 | 0.03617689E-01 | -0.02726208E-04 | 0.01877183E-07  | -0.12591780E-11 | 0.12482649E+06 | -0.13091947E+02 |
| 0600-1500K   | 0.13568498E+02 | 0.02802435E-01 | -0.07969918E-05 | -0.06437098E-08 | 0.15602546E-12  | 0.12480055E+06 | -0.13810628E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

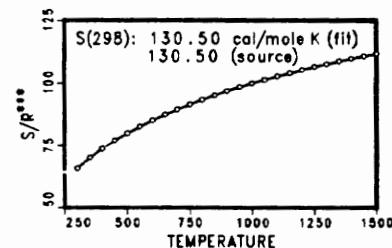
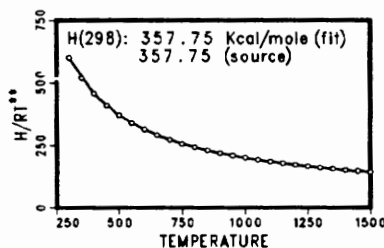
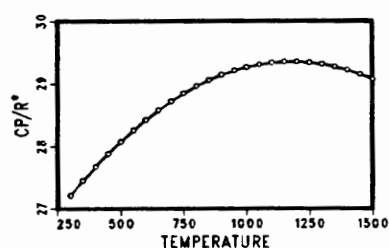
Species: GAAS(5,C)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-0600K   | 0.02546511E+03 | 0.07014337E-01 | -0.04881356E-04 | 0.03825484E-07  | -0.02450420E-10 | 0.01721819E+07 | -0.08130267E+03 |
| 0600-1500K   | 0.02573672E+03 | 0.05523956E-01 | -0.12034680E-05 | -0.10437431E-08 | 0.02528930E-11  | 0.01721381E+07 | -0.08254488E+03 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

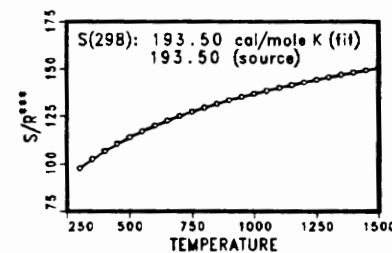
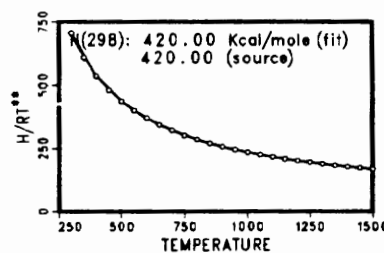
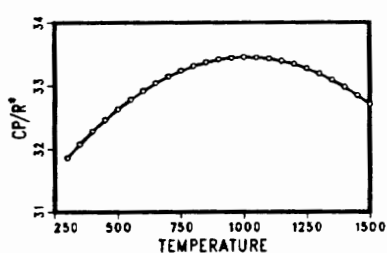
Species: GAAS(5,L)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-0600K   | 0.03015255E+03 | 0.07234394E-01 | -0.06497993E-04 | 0.05559584E-07  | -0.03339653E-10 | 0.02021150E+07 | -0.07630866E+03 |
| 0600-1500K   | 0.03045793E+03 | 0.05403151E-01 | -0.16494765E-05 | -0.09968843E-08 | 0.02413154E-11  | 0.02020691E+07 | -0.07768010E+03 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: GAET

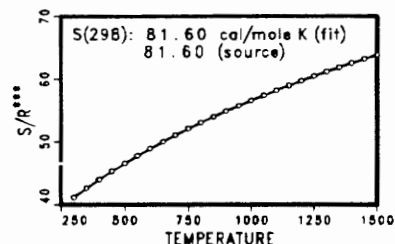
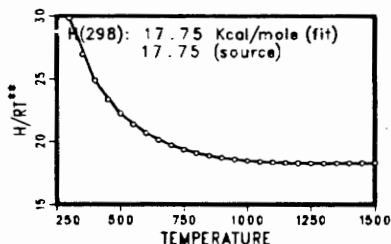
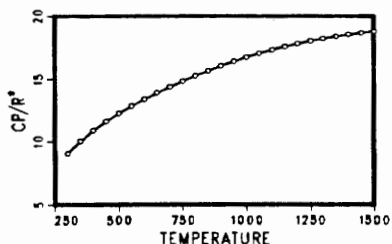
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.01846399E+02 | 0.02592050E+00 | 0.05522393E-04 | -0.04977960E-06 | 0.03654361E-09 | 0.07264445E+05 | 0.02294638E+03 |
| 0600-1500K   | 0.05932970E+02 | 0.13424544E-01 | 0.04110518E-05 | -0.04286069E-07 | 0.12387095E-11 | 0.06504863E+05 | 0.03090838E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2/T + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: GAET2

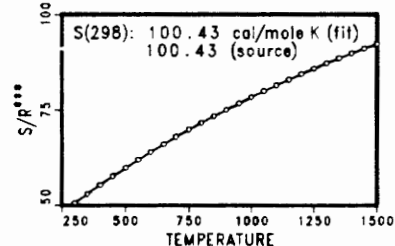
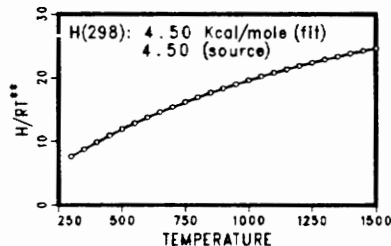
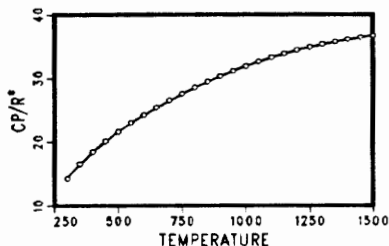
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.02162930E+02 | 0.05892512E+00 | 0.14471449E-04 | -0.11686023E-06 | 0.08526654E-09 | 0.03561840E+04  | 0.04552626E+03  |
| 0600-1500K   | 0.07213832E+02  | 0.03055227E+00 | 0.12494508E-05 | -0.09990274E-07 | 0.02881965E-10 | -0.13921194E+04 | -0.07795098E+00 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2/T + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: GAET3

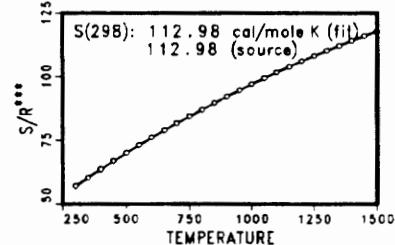
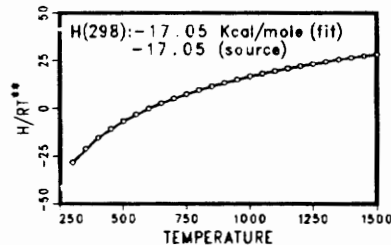
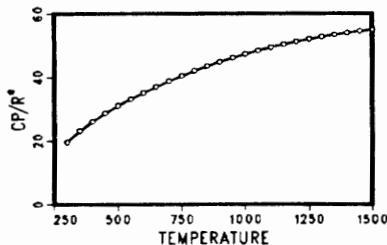
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.06544288E+02 | 0.09332246E+00 | 0.02364121E-03 | -0.01874104E-05 | 0.13677210E-09 | -0.10676594E+05 | 0.06666796E+03  |
| 0600-1500K   | 0.08436453E+02  | 0.04804950E+00 | 0.02119157E-04 | -0.15816849E-07 | 0.04571178E-10 | -0.13469963E+05 | -0.06196490E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2/T + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

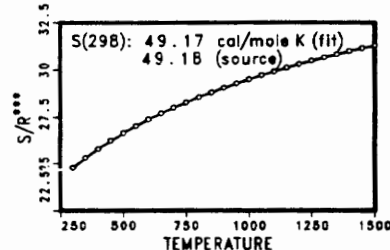
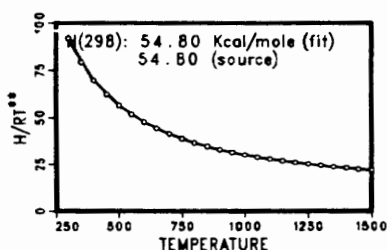
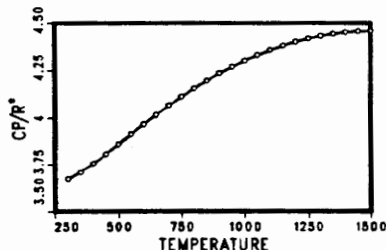
Species: GAH

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-0600K   | 0.03524579E+02 | 0.03386213E-02 | -0.02064013E-05 | 0.03220998E-07  | -0.02936132E-10 | 0.02651074E+06 | 0.04554066E+02 |
| 0600-1500K   | 0.03232142E+02 | 0.13432469E-02 | -0.04325498E-06 | -0.02791841E-08 | 0.04973590E-12  | 0.02656059E+06 | 0.05947896E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

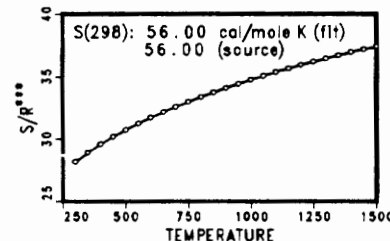
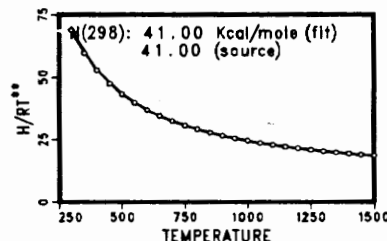
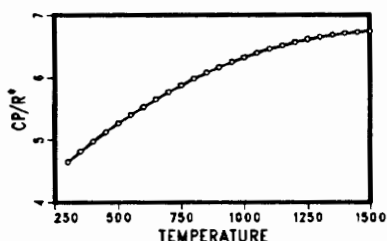
Species: GAH2

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.03559710E+02 | 0.03676741E-01 | 0.06484499E-05 | -0.03109349E-07 | 0.15854136E-11 | 0.01940976E+06 | 0.06803081E+02 |
| 0600-1500K   | 0.03762384E+02 | 0.03210792E-01 | 0.02180096E-06 | -0.08908394E-08 | 0.02219062E-11 | 0.01936646E+06 | 0.05783398E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

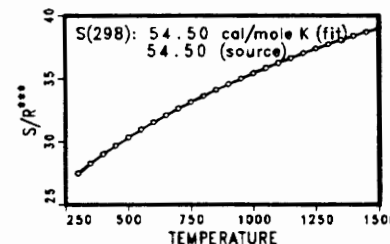
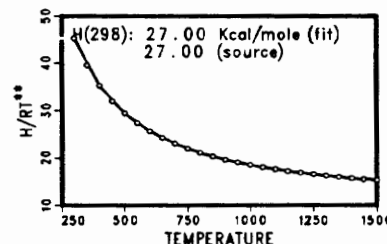
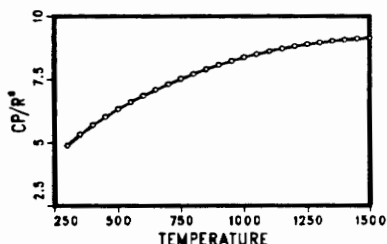
Species: GAH3

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.01726153E+02 | 0.11247386E-01 | 0.02447526E-04 | -0.02026314E-06 | 0.14470000E-10 | 0.12586196E+05 | 0.14284450E+02 |
| 0600-1500K   | 0.03345475E+02 | 0.06399313E-01 | 0.11229964E-06 | -0.02065899E-07 | 0.05780202E-11 | 0.12281851E+05 | 0.06394841E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: GAME

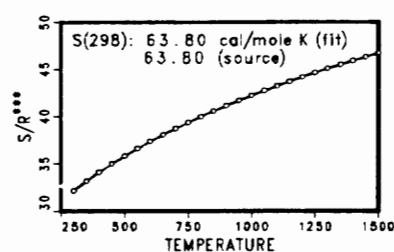
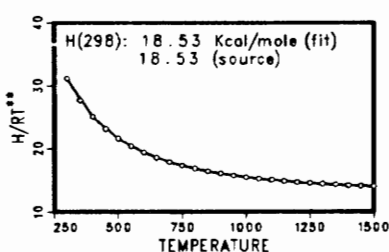
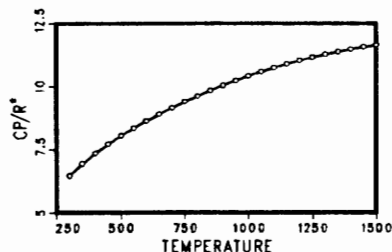
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.03054536E+02 | 0.12186402E-01 | 0.02332213E-04 | -0.02121866E-06 | 0.15442261E-10 | 0.07885868E+05 | 0.11128781E+02 |
| 0600-1500K   | 0.04809857E+02 | 0.06824206E-01 | 0.02258235E-05 | -0.02018341E-07 | 0.05736453E-11 | 0.07558677E+05 | 0.02595904E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: GAME2

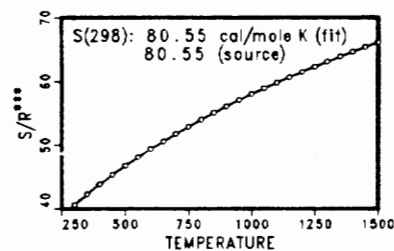
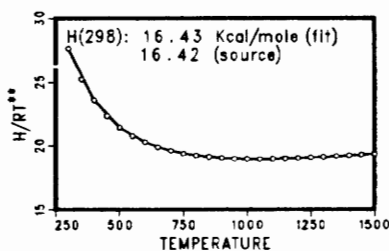
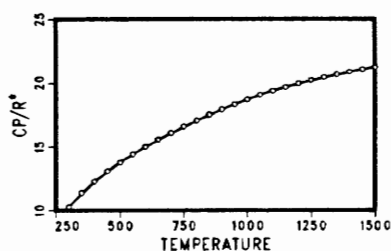
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|
| 0300-0600K   | 0.02257655E+02 | 0.02916445E+00 | 0.05669861E-04 | -0.05709755E-06 | 0.042688905E-09 | 0.06341297E+05 | 0.01915435E+03  |
| 0600-1500K   | 0.07068372E+02 | 0.14216021E-01 | 0.05120694E-05 | -0.04421986E-07 | 0.13096413E-11  | 0.05453790E+05 | -0.04173960E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: GAME3

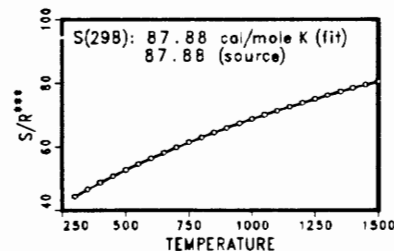
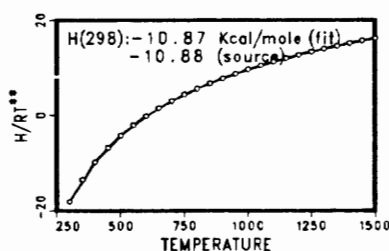
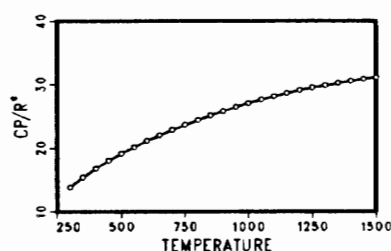
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | 0.02120238E+02 | 0.04161029E+00 | 0.09959505E-04 | -0.07846792E-06 | 0.05693396E-09 | -0.07911968E+05 | 0.01988516E+03  |
| 0600-1500K   | 0.08410636E+02 | 0.02262803E+00 | 0.10430190E-05 | -0.07049610E-07 | 0.02015307E-10 | -0.09087271E+05 | -0.10722496E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: H

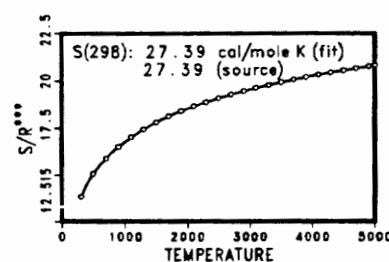
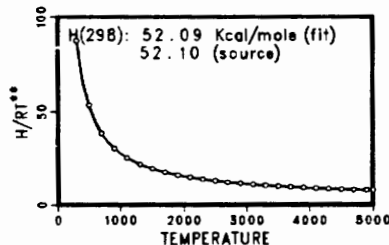
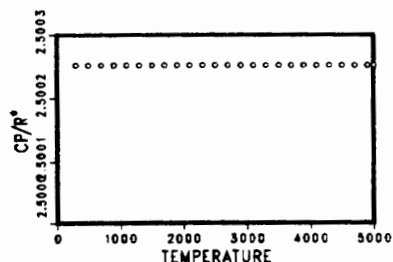
HYDROGEN, MONATOMIC

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.02547162E+06 | -0.04601176E+01 |
| 1000-5000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.02547162E+06 | -0.04601176E+01 |



Source: NASA FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H+

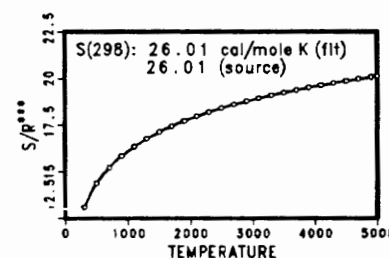
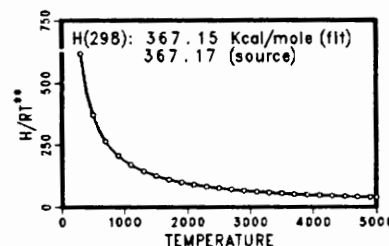
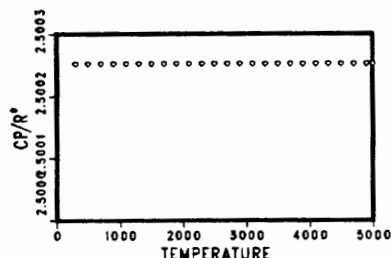
PROTON

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.01840334E+07 | -0.11538621E+01 |
| 1000-5000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.01840334E+07 | -0.11538620E+01 |



Source: NASA FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H-

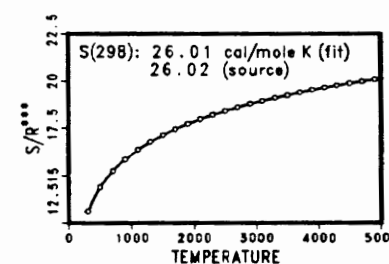
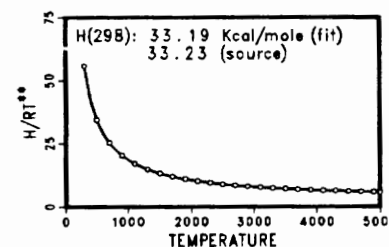
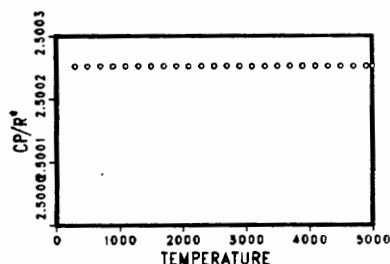
HYDROGEN, UNINEGATIVE ION

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.15961045E+05 | -0.11524486E+01 |
| 1000-5000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.15961045E+05 | -0.11524488E+01 |



Source: NASA FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



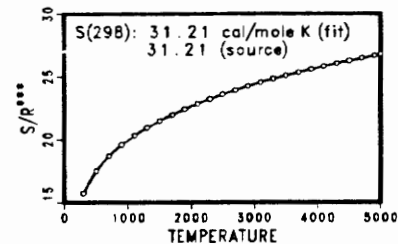
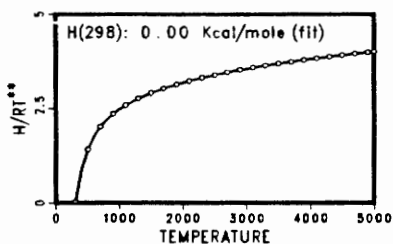
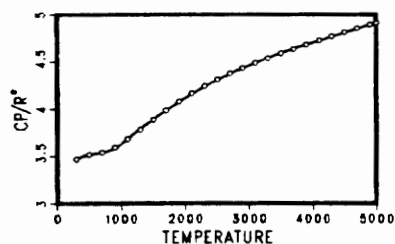
Species: H2

HYDROGEN, DIATOMIC (REF ST) GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.03298124E+02 | 0.08249441E-02 | -0.08143015E-05 | -0.09475434E-09 | 0.04134872E-11 | -0.10125209E+04 | -0.03294094E+02 |
| 1000-5000K   | 0.02991423E+02 | 0.07000644E-02 | -0.05633828E-06 | -0.09231578E-10 | 0.15827519E-14 | -0.08350340E+04 | -0.13551101E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2ALME

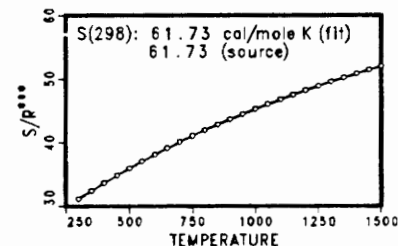
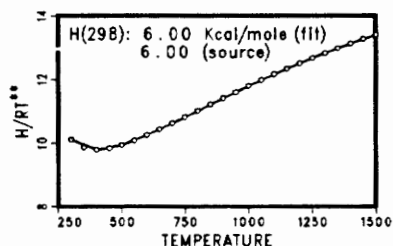
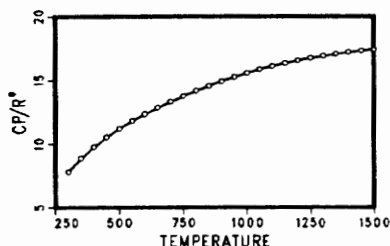
("ME" = CH3,METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | -0.06283259E+01 | 0.03089530E+00 | 0.05774090E-04 | -0.06488033E-06 | 0.04907111E-09 | 0.01889333E+05 | 0.02565779E+03  |
| 0600-1500K   | 0.04898410E+02  | 0.13582233E-01 | 0.02611458E-05 | -0.04575170E-07 | 0.13848023E-11 | 0.08743072E+04 | -0.11131169E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2ASME

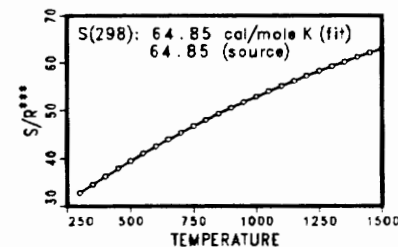
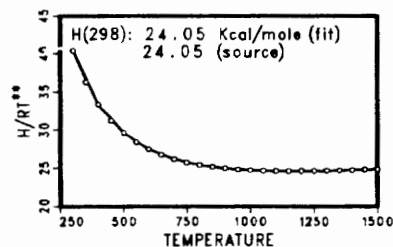
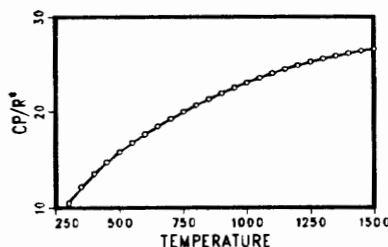
("ME" = CH3,METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | -0.02113506E+02 | 0.04564229E+00 | 0.09983227E-04 | -0.09399697E-06 | 0.07014021E-09 | 0.10771701E+05 | 0.03132610E+03  |
| 0600-1500K   | 0.05686213E+02  | 0.02154421E+00 | 0.08185247E-05 | -0.07069951E-07 | 0.02101522E-10 | 0.09331084E+05 | -0.06513957E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2C4O

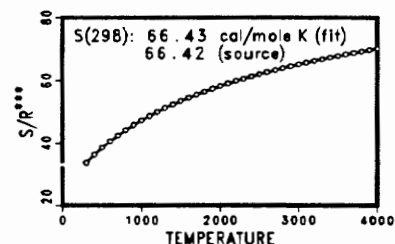
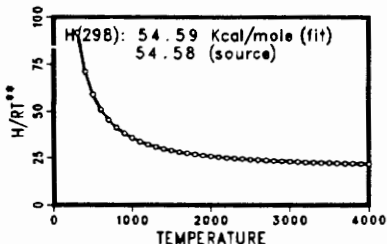
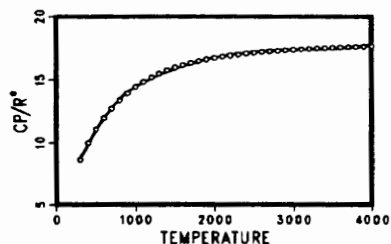
BUTADIENONE

GAS

As of: 12/01/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.04810971E+02 | 0.13139968E-01 | 0.09865073E-05  | -0.06120720E-07 | 0.16400028E-11 | 0.02545803E+06 | 0.02113424E+02  |
| 1000-4000K   | 0.10268878E+02 | 0.04896164E-01 | -0.04885080E-05 | -0.02708566E-08 | 0.05107013E-12 | 0.02346902E+06 | -0.02815985E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

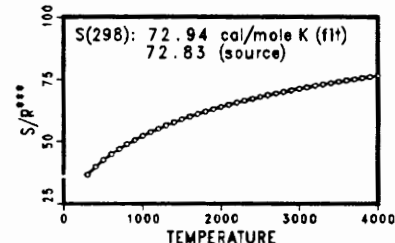
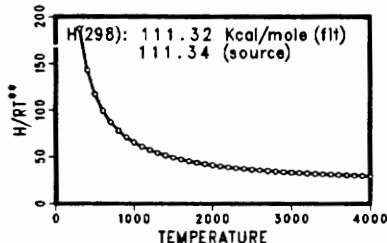
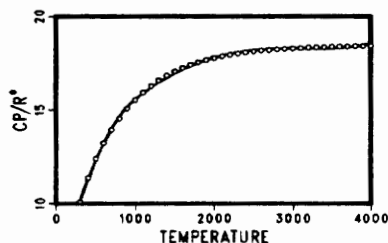
Species: H2CCCCH

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.06545799E+02 | 0.12424768E-01 | 0.05603226E-05  | -0.05631141E-07 | 0.16652183E-11 | 0.05352502E+06 | -0.04264082E+02 |
| 1000-4000K   | 0.11314095E+02 | 0.05014414E-01 | -0.05350444E-05 | -0.02825309E-08 | 0.05403279E-12 | 0.05181211E+06 | -0.03062434E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2CCCCH2

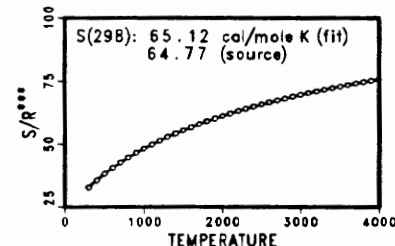
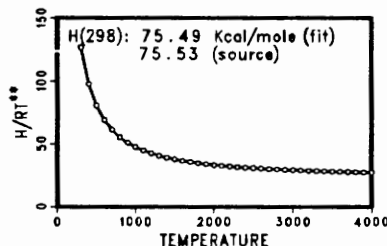
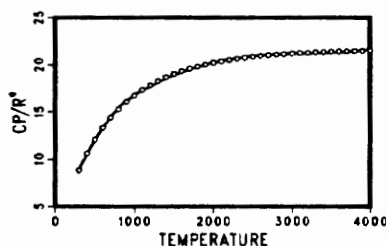
BUTATRIENE D2H

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03849007E+02 | 0.01713169E+00 | 0.16442703E-05  | -0.07761590E-07 | 0.01947859E-10 | 0.03608372E+06 | 0.05732120E+02  |
| 1000-4000K   | 0.10620828E+02 | 0.07199370E-01 | -0.06806234E-05 | -0.04021185E-08 | 0.07378498E-12 | 0.03358797E+06 | -0.03193583E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2CCCH

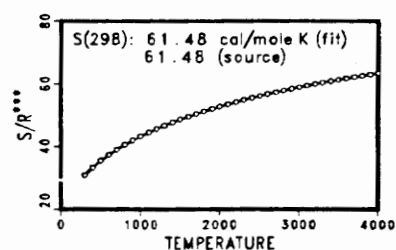
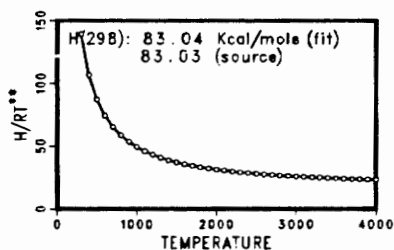
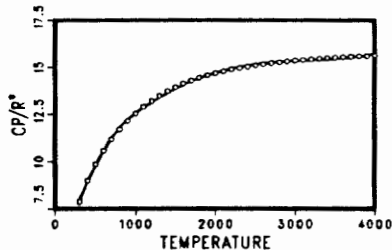
2-PROPYNYL C2V 2B2

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.04754199E+02 | 0.11080277E-01 | 0.02793323E-05  | -0.05479212E-07 | 0.01949629E-10 | 0.03988883E+06 | 0.05854549E+01  |
| 1000-4000K   | 0.08831047E+02 | 0.04357194E-01 | -0.04109066E-05 | -0.02368723E-08 | 0.04376520E-12 | 0.03847419E+06 | -0.02177919E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

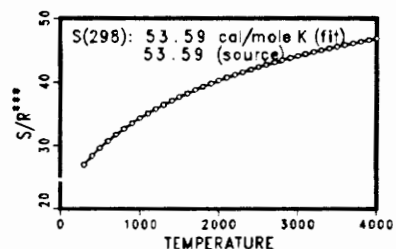
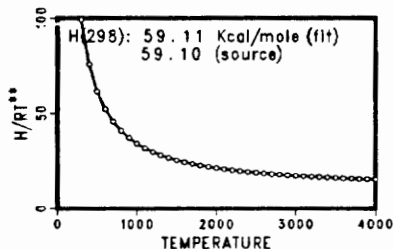
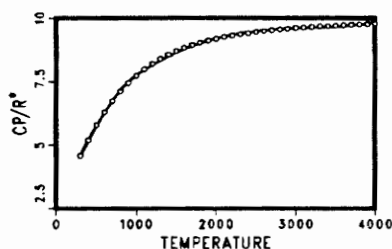
Species: H2CN

GAS

As of: 4/16/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02851661E+02 | 0.05695233E-01 | 0.10711403E-05  | -0.16226120E-08 | -0.02351108E-11 | 0.02863782E+06 | 0.08992751E+02  |
| 1000-4000K   | 0.05209703E+02 | 0.02969291E-01 | -0.02855589E-05 | -0.16355504E-09 | 0.03043259E-12  | 0.02767711E+06 | -0.04444478E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

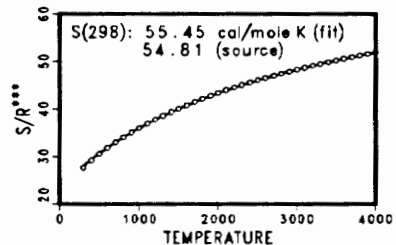
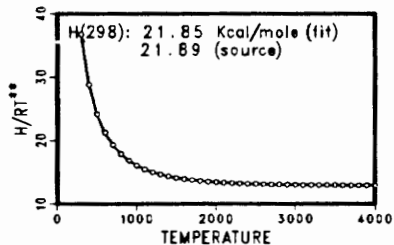
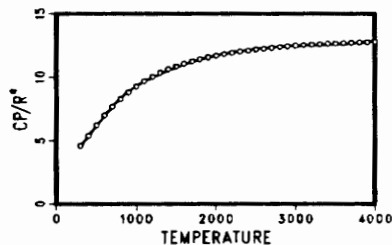
Species: H2CNH

GAS

As of: 4/16/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02365878E+02 | 0.06780570E-01 | 0.02422999E-04  | -0.06157824E-08 | -0.16150971E-11 | 0.09971141E+05 | 0.12307176E+02  |
| 1000-4000K   | 0.05221589E+02 | 0.04748525E-01 | -0.04179158E-05 | -0.02606612E-08 | 0.04703140E-12  | 0.08657219E+05 | -0.04500776E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

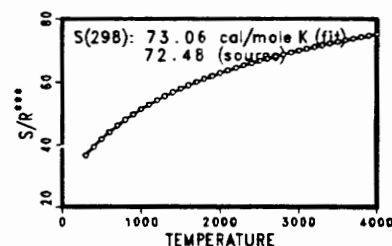
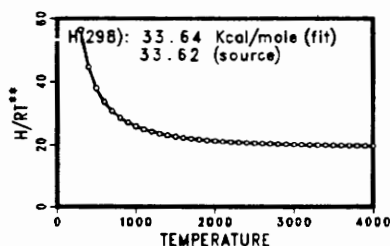
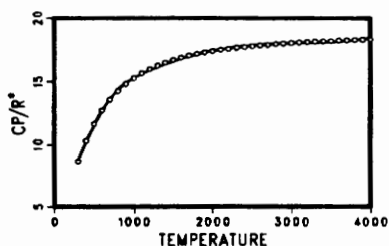
Species: H2CNN02

GAS

As of: 4/16/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03534316E+02 | 0.01811271E+00 | 0.02394017E-05  | -0.10800240E-07 | 0.04222725E-10 | 0.15090057E+05 | 0.11311378E+02  |
| 1000-4000K   | 0.11407942E+02 | 0.04564542E-01 | -0.04600304E-05 | -0.02513538E-08 | 0.04782211E-12 | 0.12421422E+05 | -0.03165237E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: H2GAET

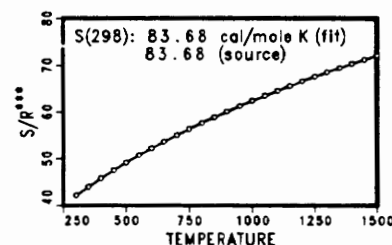
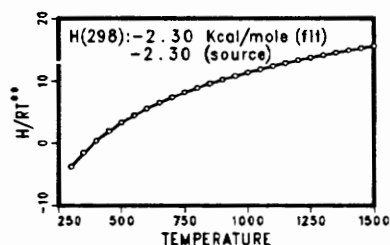
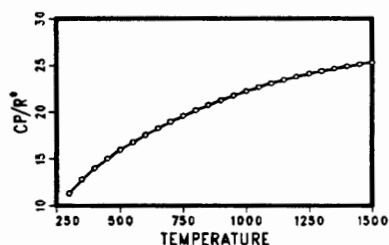
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | 0.04124020E+01 | 0.03972971E+00 | 0.07979140E-04 | -0.08059233E-06 | 0.06040387E-09 | -0.02983932E+05 | 0.02816147E+03  |
| 0600-1500K   | 0.07187273E+02 | 0.01867211E+00 | 0.06156157E-05 | -0.06027763E-07 | 0.01797524E-10 | -0.04232757E+05 | -0.04686699E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: H2GAME

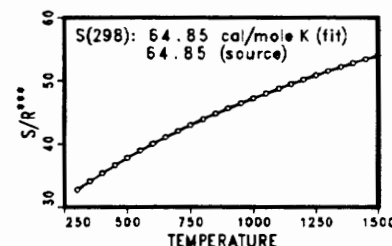
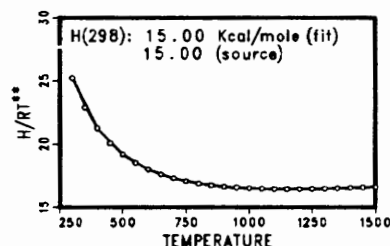
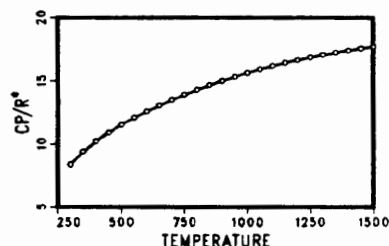
("ME" = CH3, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.05251130E+01 | 0.02904695E+00 | 0.04844148E-04 | -0.06097646E-06 | 0.04672763E-09 | 0.06158712E+05 | 0.02122148E+03  |
| 0600-1500K   | 0.05831604E+02 | 0.12228715E-01 | 0.03033669E-05 | -0.03956941E-07 | 0.12254516E-11 | 0.05189255E+05 | -0.04446614E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: H2NF

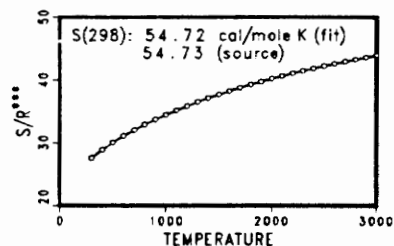
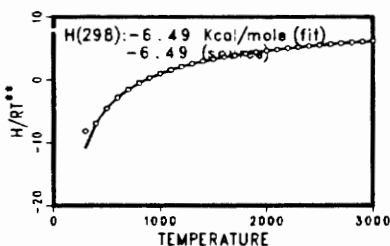
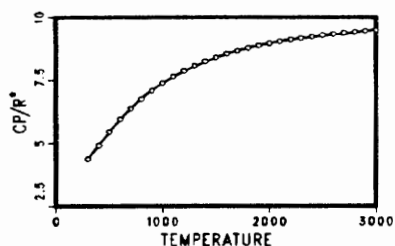
FLUOROAMMONIA

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|----------------|
| 0300-1000K   | 0.02597862E+02 | 0.05882104E-01 | 0.04938351E-05  | -0.01948600E-07 | 0.03634002E-11 | -0.04301253E+05 | 0.10982895E+02 |
| 1000-3000K   | 0.04143658E+02 | 0.03805135E-01 | -0.02771153E-05 | -0.03589717E-08 | 0.07589549E-12 | -0.04891486E+05 | 0.02309362E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2O

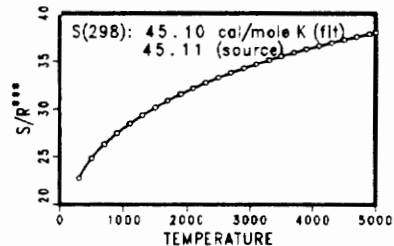
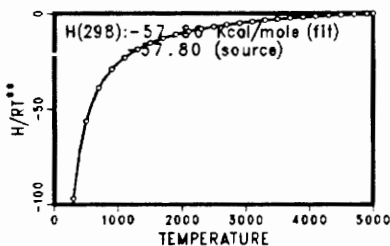
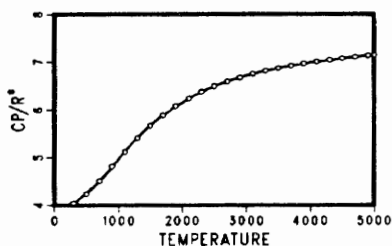
WATER

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03386842E+02 | 0.03474982E-01 | -0.06354696E-04 | 0.06968581E-07 | -0.02506588E-10 | -0.03020811E+06 | 0.02590232E+02 |
| 1000-5000K   | 0.02672145E+02 | 0.03056293E-01 | -0.08730260E-05 | 0.12009964E-09 | -0.06391618E-13 | -0.02989921E+06 | 0.06862817E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2O(L)

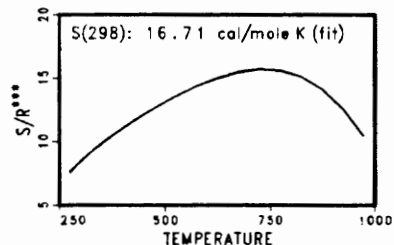
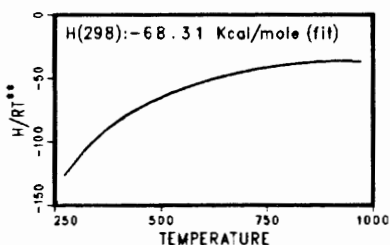
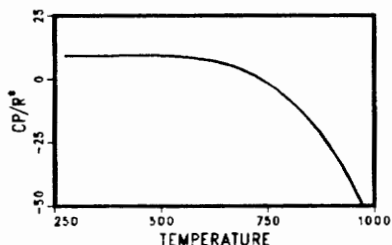
WATER

LIQUID

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0273-1000K   | 0.12712782E+02 | -0.01766279E+00 | -0.02255666E-03 | 0.02082090E-05 | -0.02407861E-08 | -0.03748320E+06 | -0.05911534E+03 |
| 1000-1000K   | 0.00000000E+00 | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00  | 0.00000000E+00  | 0.00000000E+00  |



Source: NASA FIT TO NASA LEWIS DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2O(S)

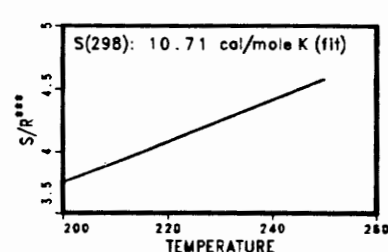
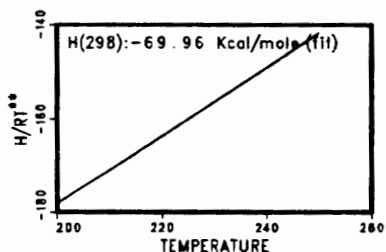
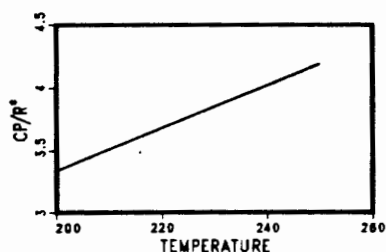
WATER

SOLID

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|-----------------|----------------|----------------|----------------|----------------|-----------------|----------------|
| 0200-1000K   | -0.03926933E+00 | 0.01692042E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | -0.03594958E+06 | 0.05693378E+01 |
| 1000-0273K   | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00  | 0.00000000E+00 |



Source: NASA FIT TO NASA LEWIS DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2O2

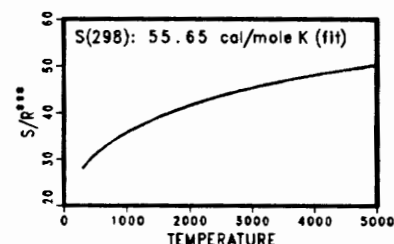
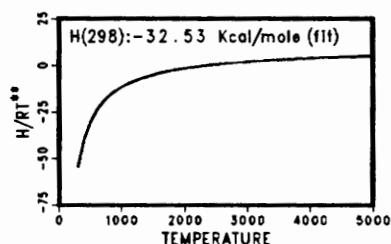
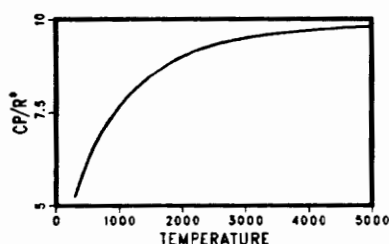
HYDROGEN PEROXIDE

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03388753E+02 | 0.06569226E-01 | -0.14850125E-06 | -0.04625805E-07 | 0.02471514E-10  | -0.01766314E+06 | 0.06785363E+02 |
| 1000-5000K   | 0.04573167E+02 | 0.04336136E-01 | -0.14746888E-05 | 0.02348903E-08  | -0.14316536E-13 | -0.01800696E+06 | 0.05011369E+01 |



Source: NASA FIT TO NASA-LEWIS DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2S

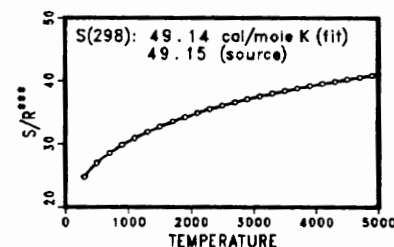
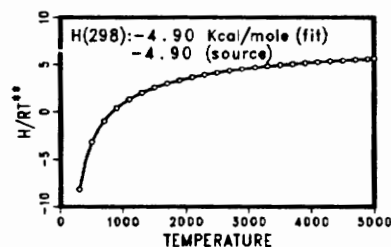
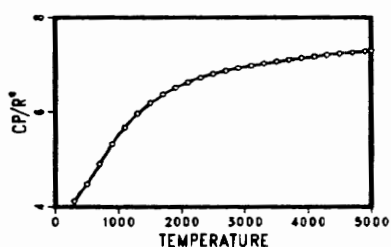
HYDROGEN SULFIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03071029E+02 | 0.05578261E-01 | -0.10309669E-04 | 0.12019529E-07 | -0.04838369E-10 | -0.03559826E+05 | 0.05935226E+02 |
| 1000-5000K   | 0.02883147E+02 | 0.03827835E-01 | -0.14233978E-05 | 0.02497998E-08 | -0.16602733E-13 | -0.03480742E+05 | 0.07258161E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2Si(NH2)2

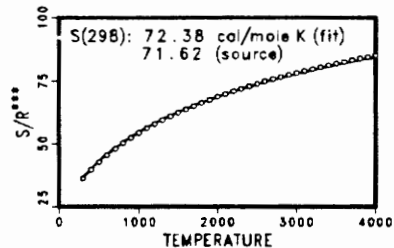
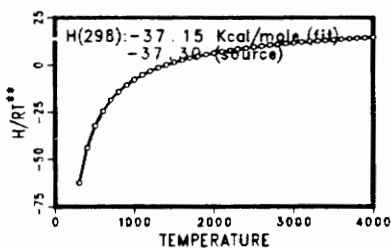
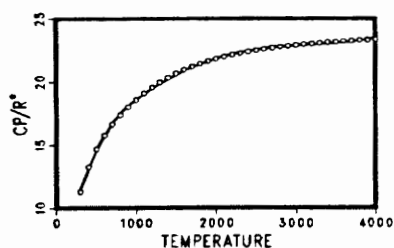
DIAMINOSILANE

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.05615307E+02 | 0.02079854E+00 | -0.09999531E-05 | -0.12885246E-07 | 0.06091865E-10 | -0.02126283E+06 | -0.16156578E+01 |
| 1000-4000K   | 0.13021791E+02 | 0.06465444E-01 | -0.05816746E-05 | -0.03484493E-08 | 0.06340675E-12 | -0.02357070E+06 | -0.04132569E+03 |



Source: SNL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

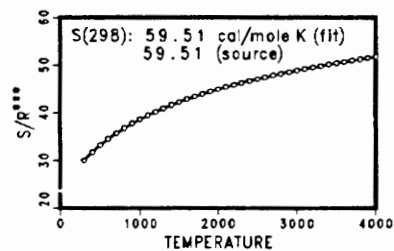
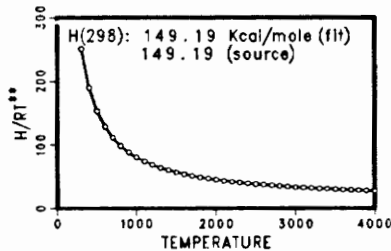
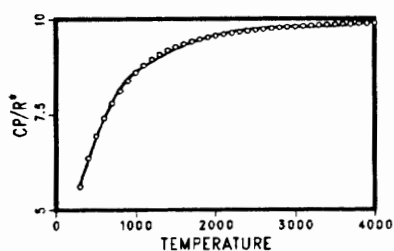
Species: H2SIN

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03549344E+02 | 0.07311004E-01 | 0.03249025E-05  | -0.03682945E-07 | 0.11215113E-11 | 0.07370656E+06 | 0.07565328E+02  |
| 1000-4000K   | 0.06826533E+02 | 0.02125460E-01 | -0.02343131E-05 | -0.11663394E-09 | 0.02277273E-12 | 0.07253672E+06 | -0.10521624E+02 |



Source: SNL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

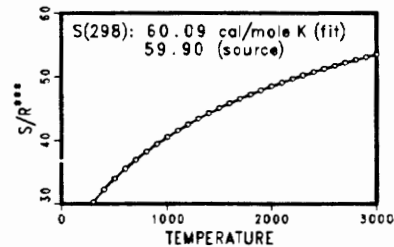
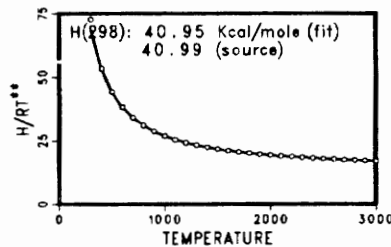
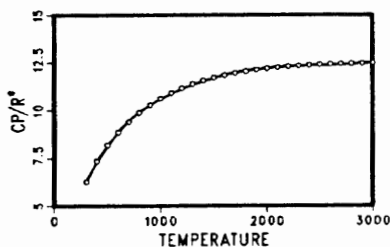
Species: H2SINH

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02822195E+02 | 0.12455182E-01 | -0.08350819E-05 | -0.07411813E-07 | 0.03579019E-10 | 0.01923616E+06 | 0.10547831E+02  |
| 1000-3000K   | 0.06588295E+02 | 0.04903194E-01 | -0.04944719E-05 | -0.05014630E-08 | 0.11394698E-12 | 0.01809794E+06 | -0.09522970E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: H2SINH2

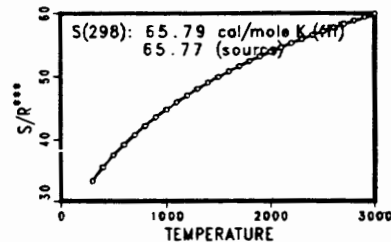
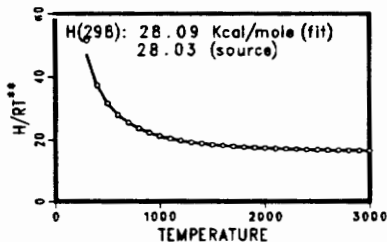
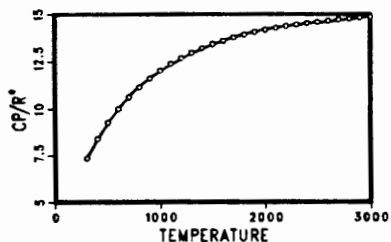
AMINOSILYL

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.04053222E+02 | 0.11822311E-01 | -0.04348128E-05 | -0.06225818E-07 | 0.02798829E-10 | 0.12419705E+05 | 0.06562032E+02  |
| 1000-3000K   | 0.07392047E+02 | 0.05476841E-01 | -0.04453276E-05 | -0.05236661E-08 | 0.11383899E-12 | 0.11368581E+05 | -0.11380495E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

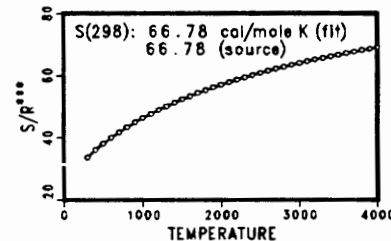
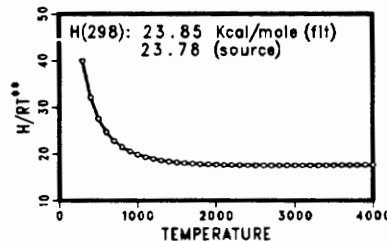
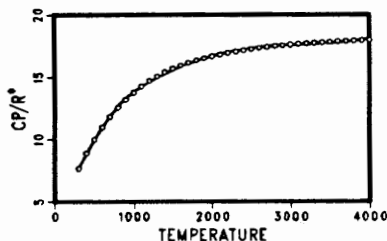
Species: H2SINH3

SILYLENE-AMMONIA TRANS STATE GAS

As of: 12/13/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04269729E+02 | 0.11252245E-01 | 0.01951721E-04  | -0.03578372E-07 | -0.08372202E-12 | 0.10222041E+05 | 0.05876735E+02  |
| 1000-4000K   | 0.08711392E+02 | 0.05909106E-01 | -0.05436615E-05 | -0.03248350E-08 | 0.05960257E-12  | 0.08441694E+05 | -0.01933470E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2SISIH2

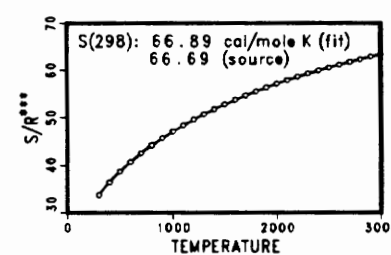
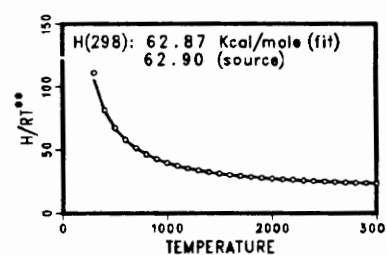
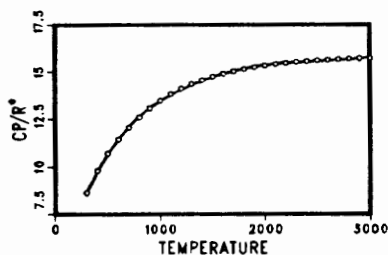
DISILENE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.05133186E+02 | 0.12528548E-01 | -0.04620421E-05 | -0.06606075E-07 | 0.02864344E-10 | 0.02956915E+06 | 0.07605133E+01  |
| 1000-3000K   | 0.08986817E+02 | 0.05405047E-01 | -0.05214021E-05 | -0.05313742E-08 | 0.11887266E-12 | 0.02832747E+06 | -0.02004478E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



Species: H3ASGAET3

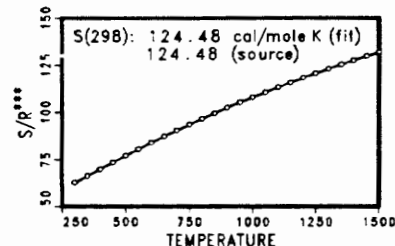
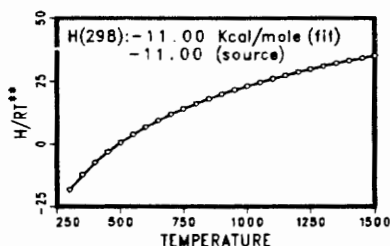
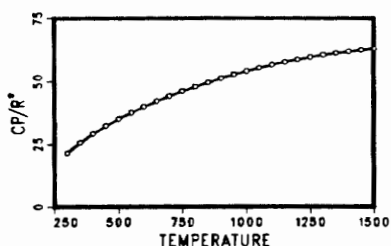
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.08974745E+02 | 0.10905161E+00 | 0.02811457E-03 | -0.02195513E-05 | 0.15997339E-09 | -0.07592761E+05 | 0.08165459E+03  |
| 0600-1500K   | 0.08508501E+02  | 0.05632369E+00 | 0.02524140E-04 | -0.01861451E-06 | 0.05372402E-10 | -0.10855169E+05 | -0.03399857E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H3ASGAME3

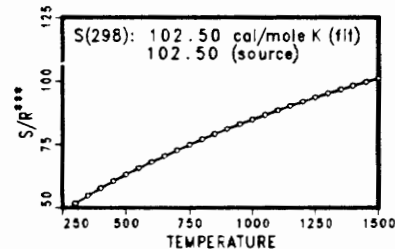
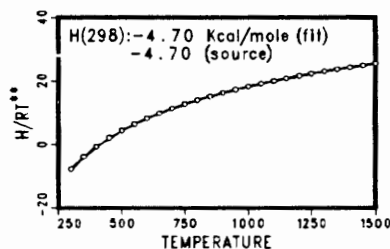
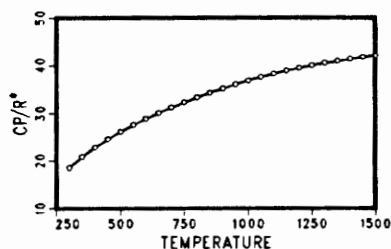
("ME" = CH3, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | 0.12671606E+01 | 0.06214586E+00 | 0.13856307E-04 | -0.12200444E-06 | 0.08982019E-09 | -0.05425619E+05 | 0.02613306E+03  |
| 0600-1500K   | 0.11254990E+02 | 0.03159752E+00 | 0.11779036E-05 | -0.10133524E-07 | 0.02947355E-10 | -0.07280344E+05 | -0.02238729E+03 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H3SIN

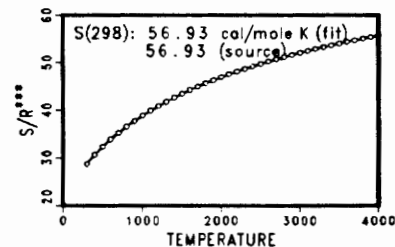
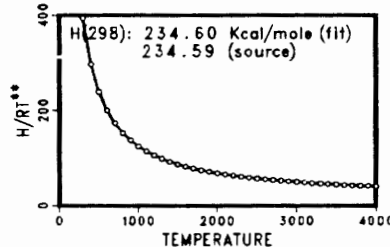
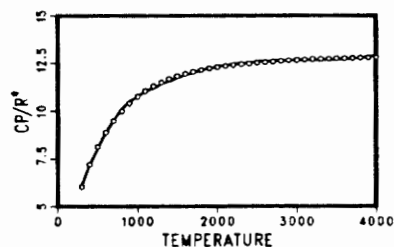
SILYLNITRENE

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02790628E+02 | 0.11345662E-01 | 0.08321879E-05  | -0.05845045E-07 | 0.01685969E-10 | 0.11673571E+06 | 0.09384630E+02  |
| 1000-4000K   | 0.07964213E+02 | 0.03355633E-01 | -0.03579695E-05 | -0.01889818E-08 | 0.03650912E-12 | 0.11486972E+06 | -0.01924110E+03 |



Source:

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H3SINH

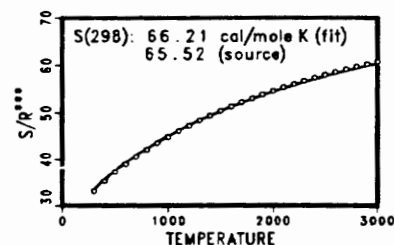
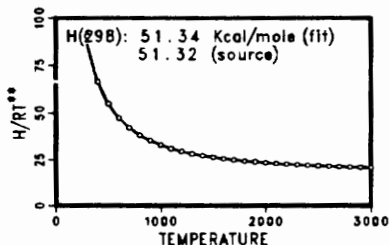
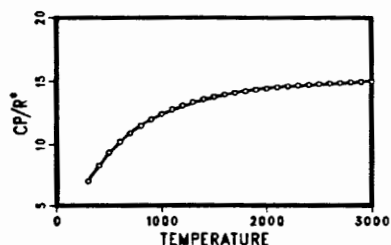
SILYLAMIDOGEN

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02778390E+02 | 0.15107111E-01 | -0.06734260E-05 | -0.08928515E-07 | 0.04115347E-10 | 0.02435913E+06 | 0.13093859E+02  |
| 1000-3000K   | 0.07697340E+02 | 0.05657943E-01 | -0.05209306E-05 | -0.05617966E-08 | 0.12635020E-12 | 0.02282005E+06 | -0.13303793E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

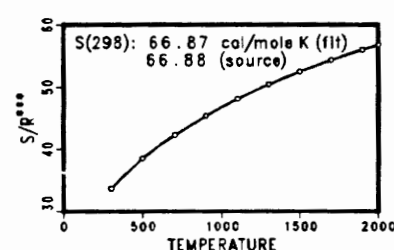
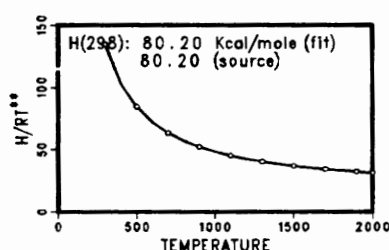
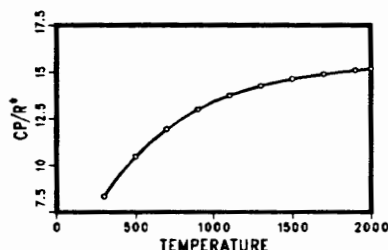
Species: H3SISIH

GAS

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02774192E+02 | 0.02555302E+00 | -0.02883836E-03 | 0.02000737E-06  | -0.06100616E-10 | 0.03861801E+06 | 0.11350098E+02  |
| 1000-2000K   | 0.07778291E+02 | 0.07255418E-01 | -0.08123265E-05 | -0.11682818E-08 | 0.03425139E-11  | 0.03742600E+06 | -0.13484629E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H3SISIH3

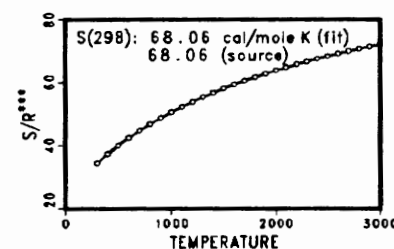
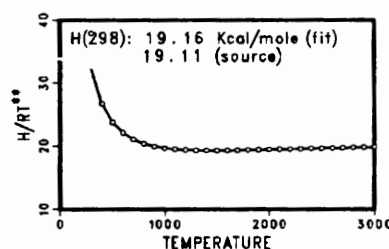
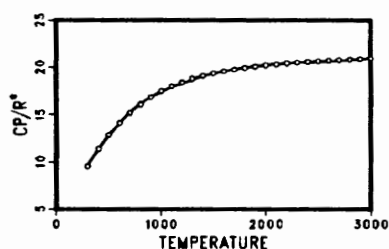
DISILANE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03898289E+02 | 0.01977415E+00 | 0.01791014E-05  | -0.10331682E-07 | 0.03931698E-10 | 0.07621719E+05 | 0.06227022E+02  |
| 1000-3000K   | 0.10682729E+02 | 0.08221416E-01 | -0.08096035E-05 | -0.08337975E-08 | 0.01908205E-11 | 0.05316920E+05 | -0.03082188E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HALME

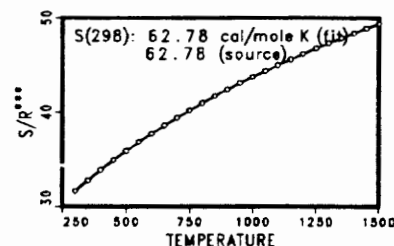
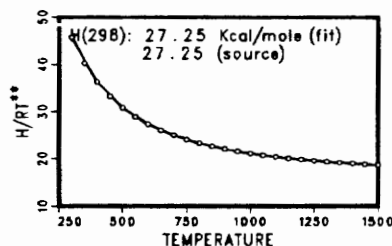
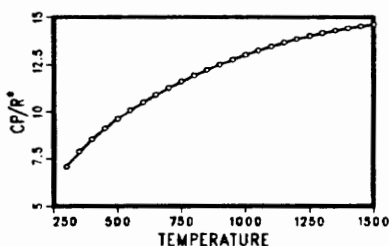
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.11187894E+01 | 0.02180038E+00 | 0.04120785E-04 | -0.04366690E-06 | 0.03273825E-09 | 0.12447363E+05 | 0.01886107E+03 |
| 0600-1500K   | 0.04812273E+02 | 0.10296448E-01 | 0.02582807E-05 | -0.03323596E-07 | 0.09884584E-11 | 0.11766730E+05 | 0.09557062E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HALME2

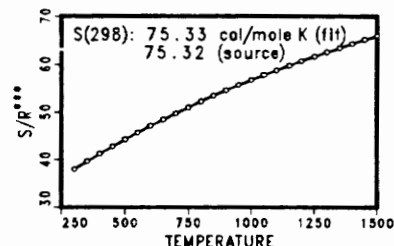
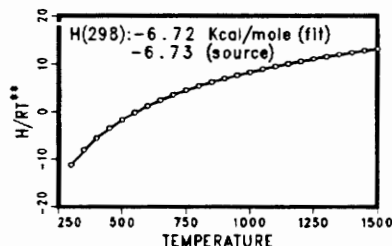
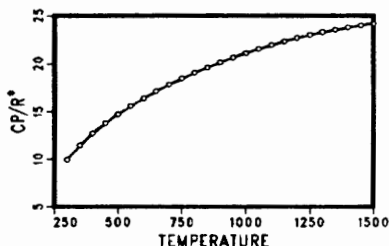
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.14942614E+01 | 0.04158567E+00 | 0.08686772E-04 | -0.08604142E-06 | 0.06447652E-09 | -0.04722516E+05 | 0.03427724E+03  |
| 0600-1500K   | 0.05705171E+02  | 0.01924317E+00 | 0.06377855E-05 | -0.06346800E-07 | 0.01896799E-10 | -0.06049864E+05 | -0.06331378E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASALME

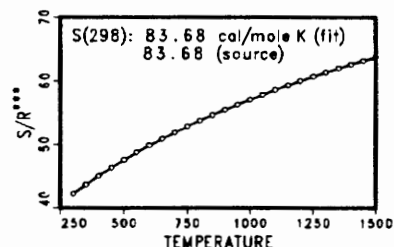
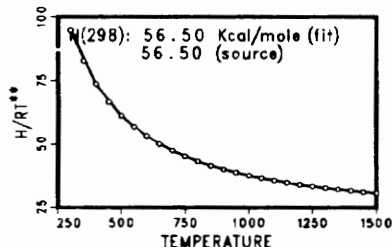
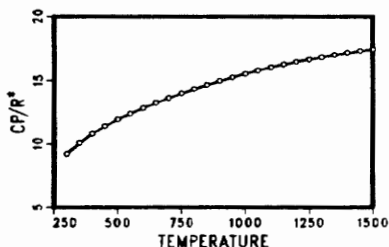
("ME" = CH<sub>3</sub>METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.02544858E+02 | 0.02465794E+00 | 0.03677807E-04 | -0.05008893E-06 | 0.03848383E-09 | 0.02663010E+06 | 0.02046858E+03  |
| 0600-1500K   | 0.06956538E+02 | 0.10612781E-01 | 0.02440153E-05 | -0.03297737E-07 | 0.10200039E-11 | 0.02582505E+06 | -0.08625792E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASGAET

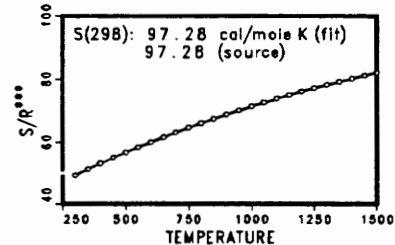
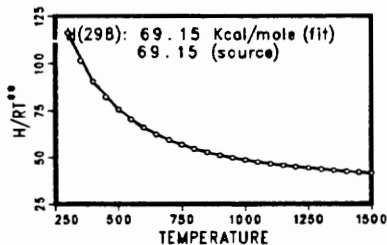
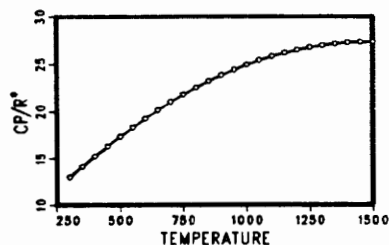
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | 0.05642723E+02 | 0.02296738E+00 | 0.10948674E-04 | -0.02449038E-06 | 0.09602700E-10 | 0.03204717E+06 | 0.09675533E+02 |
| 0600-1500K   | 0.06336445E+02 | 0.02340603E+00 | 0.09066638E-05 | -0.07519059E-07 | 0.01828115E-10 | 0.03184605E+06 | 0.05812180E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASGAME

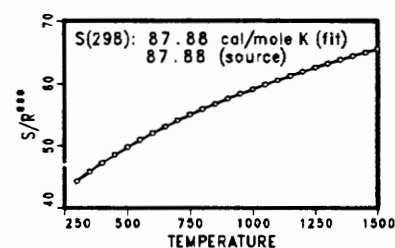
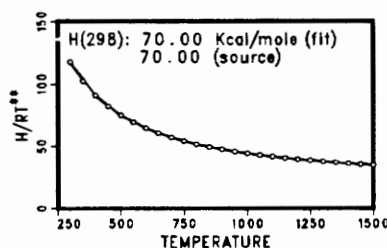
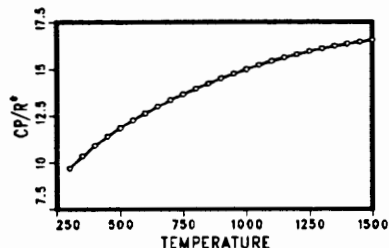
("ME" = CH3, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.04859126E+02 | 0.01750423E+00 | 0.02831995E-04 | -0.03107936E-06 | 0.02299468E-09 | 0.03302941E+06 | 0.11429521E+02  |
| 0600-1500K   | 0.07507970E+02 | 0.09277900E-01 | 0.01891931E-05 | -0.02769886E-07 | 0.07996069E-11 | 0.03253907E+06 | -0.14226081E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASME

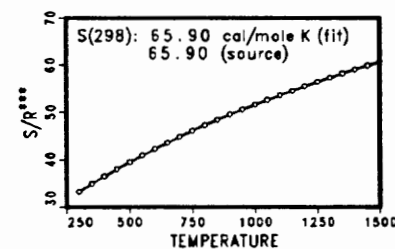
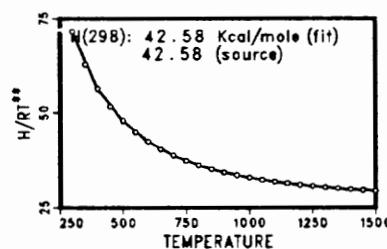
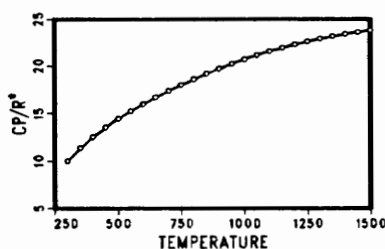
("ME" = CH3, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | -0.15750948E+00 | 0.03649094E+00 | 0.08332939E-04 | -0.07234666E-06 | 0.05330928E-09 | 0.01989791E+06 | 0.02335316E+03  |
| 0600-1500K   | 0.05753261E+02  | 0.01841813E+00 | 0.07493312E-05 | -0.05919916E-07 | 0.01726246E-10 | 0.01880057E+06 | -0.05360325E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASME2

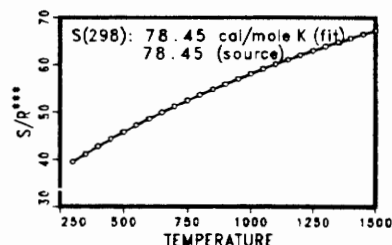
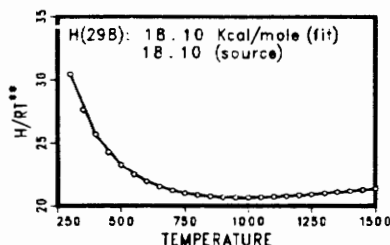
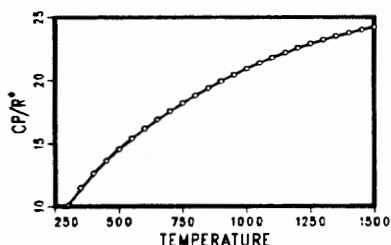
("ME" = CH3,METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|-----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | -0.02908405E+01 | 0.03729576E+00 | 0.08335854E-04 | -0.07455611E-06 | 0.05527881E-09 | 0.07587765E+05 | 0.03020451E+03 |
| 0600-1500K   | 0.05850436E+02  | 0.01841765E+00 | 0.08066844E-05 | -0.05868715E-07 | 0.01726428E-10 | 0.06450535E+05 | 0.03909152E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HCCHCCH

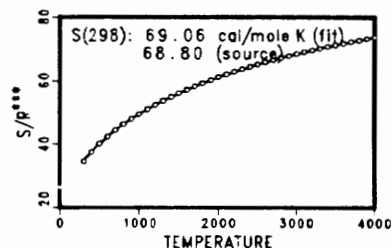
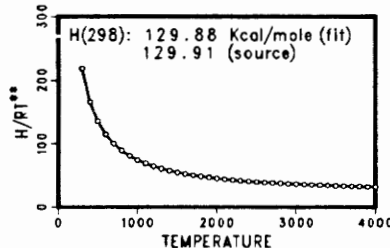
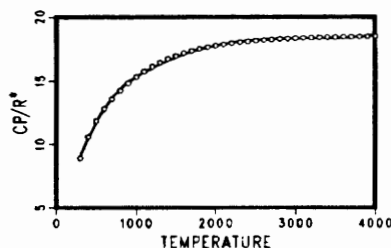
HCCH CIS

GAS

As of: 8/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.04153881E+02 | 0.01726287E+00 | -0.02389374E-05 | -0.10187000E-07 | 0.04340504E-10 | 0.06338070E+06 | 0.06036506E+02  |
| 1000-4000K   | 0.10752738E+02 | 0.05381153E-01 | -0.05549637E-05 | -0.03052266E-08 | 0.05761740E-12 | 0.06121419E+06 | -0.02973025E+03 |



Source: SNLL FIT TO BURCAT DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HCCO

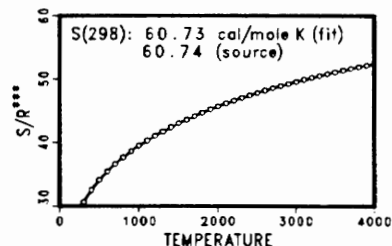
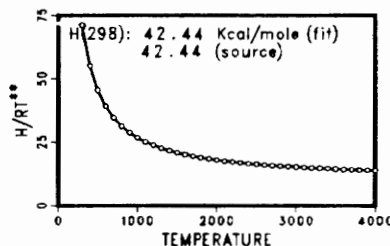
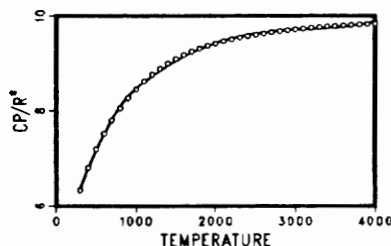
KETYL

GAS

As of: 3/23/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.05047965E+02 | 0.04453478E-01 | 0.02268282E-05  | -0.14820945E-08 | 0.02250741E-11 | 0.01965891E+06 | 0.04818439E+01  |
| 1000-4000K   | 0.06758073E+02 | 0.02000400E-01 | -0.02027607E-05 | -0.10411318E-09 | 0.01965164E-12 | 0.01901513E+06 | -0.09071262E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HCCOH

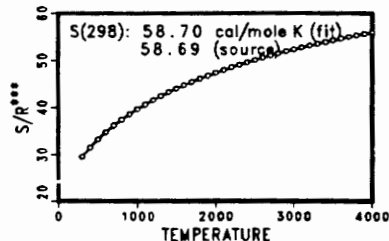
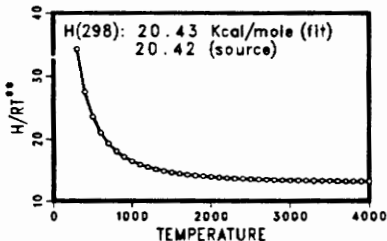
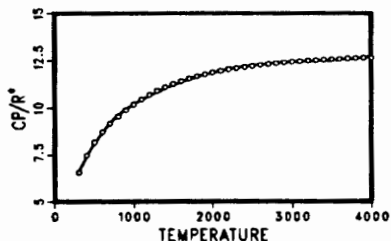
ETHYNOL

GAS

As of: 3/23/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03899465E+02 | 0.09701075E-01 | -0.03119309E-05 | -0.05537732E-07 | 0.02465732E-10 | 0.08701190E+05 | 0.04491874E+02  |
| 1000-4000K   | 0.07328324E+02 | 0.03336416E-01 | -0.03024705E-05 | -0.01781106E-08 | 0.03245168E-12 | 0.07598258E+05 | -0.14012140E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HCL

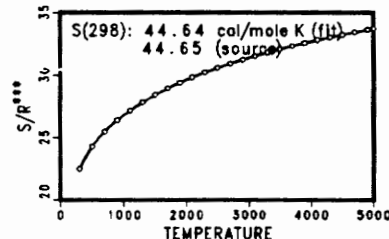
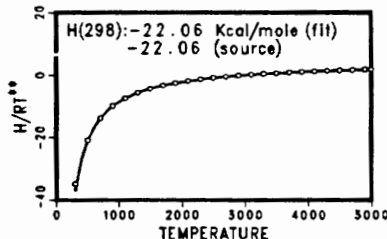
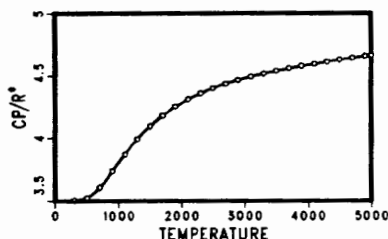
HYDROGEN CHLORIDE

GAS

As of: 4/21/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03338534E+02 | 0.12682066E-02 | -0.03666916E-04 | 0.04703992E-07 | -0.01836011E-10 | -0.12131511E+05 | 0.03193555E+02 |
| 1000-5000K   | 0.02755335E+02 | 0.14735811E-02 | -0.04971254E-05 | 0.08108658E-09 | -0.05072063E-13 | -0.11918058E+05 | 0.06515116E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HCN

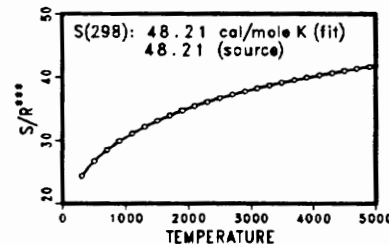
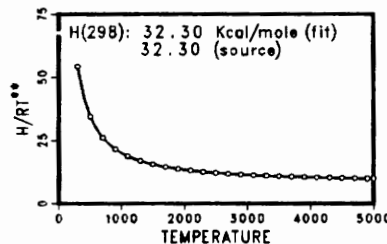
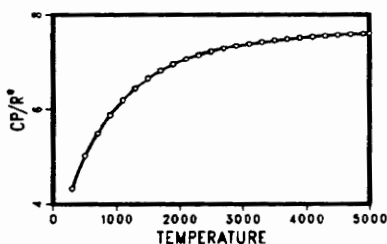
HYDROGEN CYANIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02490462E+02 | 0.08611280E-01 | -0.10310342E-04 | 0.07481498E-07 | -0.02229109E-10 | 0.15208344E+05 | 0.07904981E+02 |
| 1000-5000K   | 0.03650077E+02 | 0.03460998E-01 | -0.12742788E-05 | 0.02217655E-08 | -0.14771774E-13 | 0.14983916E+05 | 0.02393220E+02 |



Source: SNLL FIT TO JANAF TABLES (CHN)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

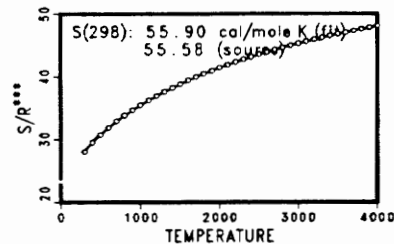
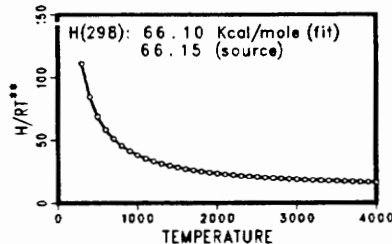
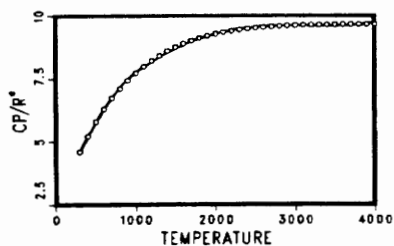
Species: HCNH

GAS

As of: 4/16/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02759456E+02 | 0.06103386E-01 | 0.07713149E-05  | -0.02063093E-07 | 0.01931919E-11 | 0.03217247E+06 | 0.10574895E+02  |
| 1000-4000K   | 0.04923292E+02 | 0.03332897E-01 | -0.03370896E-05 | -0.01901619E-08 | 0.03531825E-12 | 0.03132669E+06 | -0.16325088E+01 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

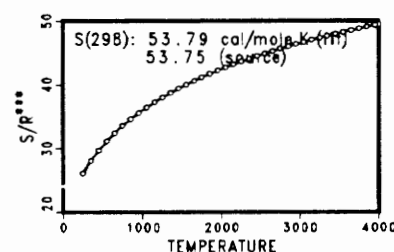
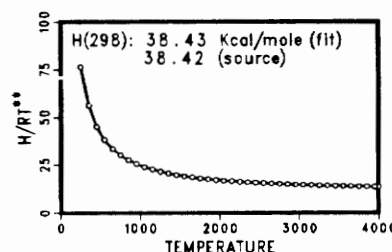
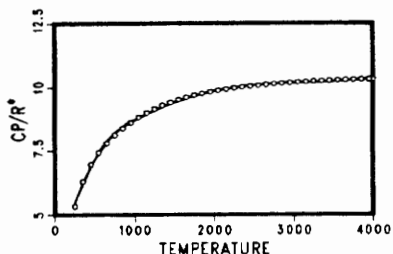
Species: HCNO

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0250-1000K   | 0.03184858E+02 | 0.09752316E-01 | -0.12802028E-05 | -0.06163104E-07 | 0.03226275E-10 | 0.01797907E+06 | 0.06123843E+02  |
| 1000-4000K   | 0.06692412E+02 | 0.02368360E-01 | -0.02371510E-05 | -0.12755033E-09 | 0.02407137E-12 | 0.01694736E+06 | -0.12454345E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HCO

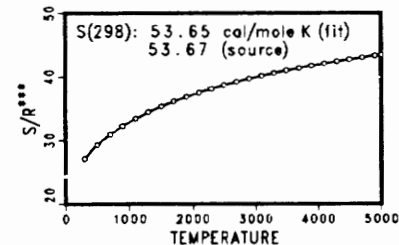
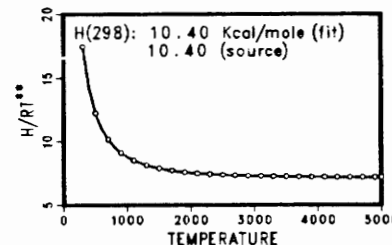
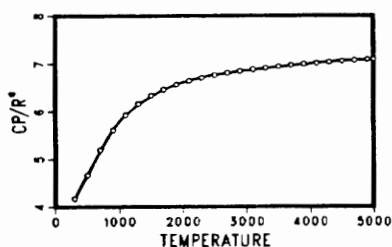
FORMYL

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02898329E+02 | 0.06199146E-01 | -0.09623084E-04 | 0.10898249E-07 | -0.04574885E-10 | 0.04159922E+05 | 0.08983614E+02 |
| 1000-5000K   | 0.03557271E+02 | 0.03345572E-01 | -0.13350060E-05 | 0.02470572E-08 | -0.01713850E-12 | 0.03916324E+05 | 0.05552299E+02 |



Source: SNLL FIT TO JANAF TABLES (CHO)

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HCO+

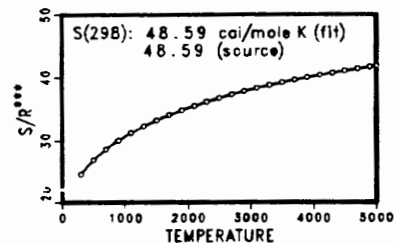
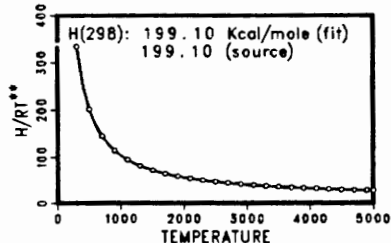
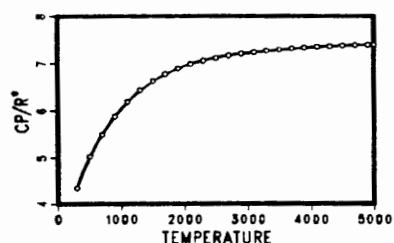
FORMYL, UNIPOSITIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02496483E+02 | 0.08690658E-01 | -0.10604453E-04 | 0.07882791E-07 | -0.02418385E-10 | 0.09915097E+06 | 0.08048177E+02 |
| 1000-5000K   | 0.03692074E+02 | 0.03454732E-01 | -0.13165244E-05 | 0.02323551E-08 | -0.15541321E-13 | 0.09890941E+06 | 0.02330722E+02 |



Source: SNLL FIT TO JANAF TABLES (CHO+)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HE

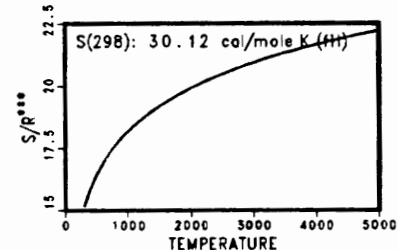
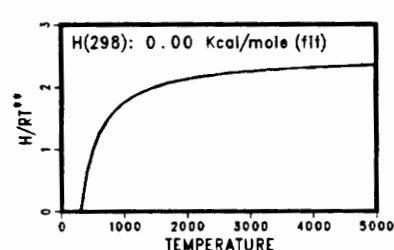
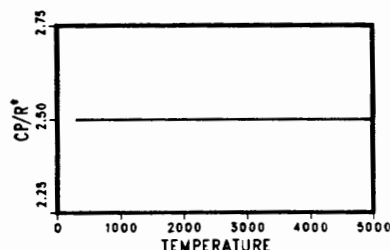
HELIUM, MONATOMIC (REF ST)

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|----------------|----------------|-----------------|----------------|
| 0300-1000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | -0.07453750E+04 | 0.09153488E+01 |
| 1000-5000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | -0.07453750E+04 | 0.09153489E+01 |



Source: NASA FIT TO NASA-LEWIS DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HE+

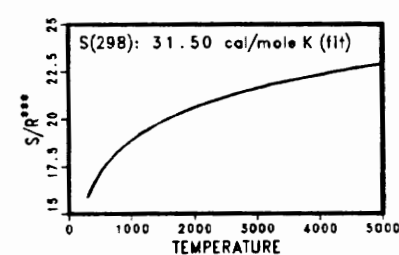
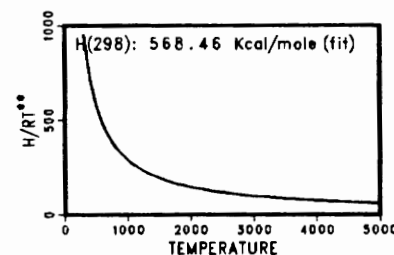
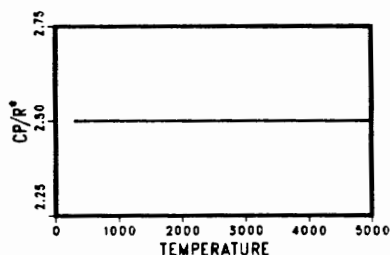
HELIUM, UNIPOSITIVE ION

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.02853426E+07 | 0.16084046E+01 |
| 1000-5000K   | 0.02500000E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.02853426E+07 | 0.16084045E+01 |



Source: NASA FIT TO NASA-LEWIS DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



Species: HF

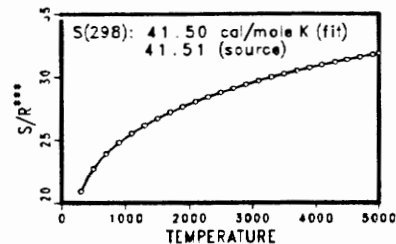
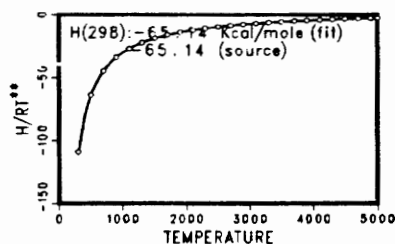
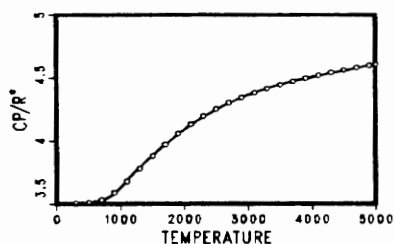
HYDROGEN FLUORIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03431841E+02 | 0.04404165E-02 | -0.08828452E-05 | 0.06574516E-08  | -0.02055909E-12 | -0.03381977E+06 | 0.12382699E+01 |
| 1000-5000K   | 0.02956767E+02 | 0.07721015E-02 | -0.09899834E-06 | -0.04993520E-10 | 0.14293306E-14  | -0.03361061E+06 | 0.04011673E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: HGAET

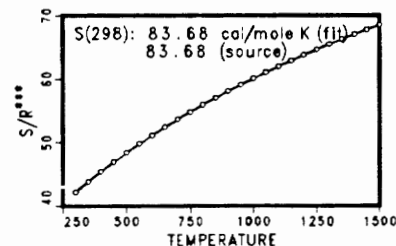
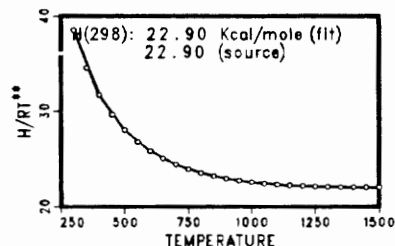
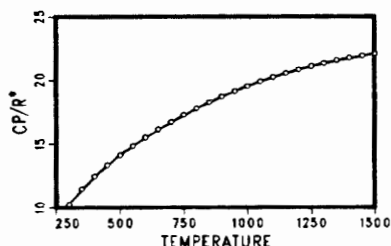
("ET" = C<sub>2</sub>H<sub>5</sub>, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.11632838E+01 | 0.03282212E+00 | 0.06765717E-04 | -0.06509541E-06 | 0.04835806E-09 | 0.09767174E+05 | 0.02588269E+03  |
| 0600-1500K   | 0.06580151E+02 | 0.16101323E-01 | 0.05009545E-05 | -0.05185148E-07 | 0.15240853E-11 | 0.08765131E+05 | -0.04046067E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: HGAET2

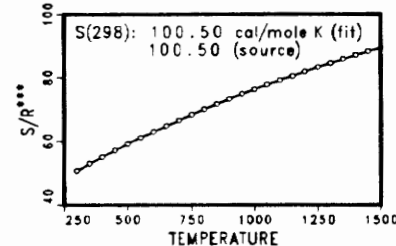
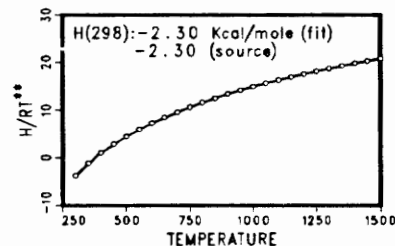
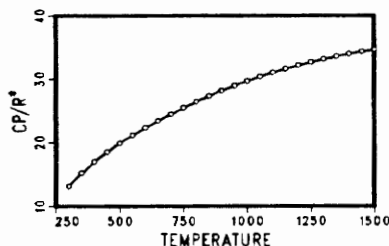
("ET" = C<sub>2</sub>H<sub>5</sub>, ETHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|----------------|
| 0300-0600K   | -0.14865759E+01 | 0.05217640E+00 | 0.13563420E-04 | -0.10119820E-06 | 0.07319853E-09 | -0.02985242E+05 | 0.04364749E+03 |
| 0600-1500K   | 0.06511306E+02  | 0.02819753E+00 | 0.14187506E-05 | -0.09000947E-07 | 0.02572894E-10 | -0.04482180E+05 | 0.04709021E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: HGAME

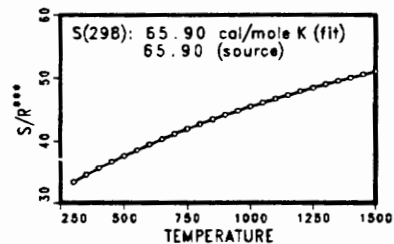
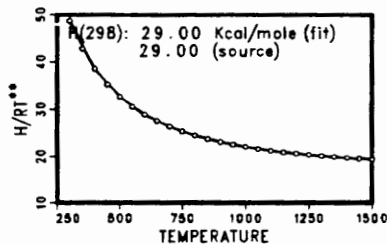
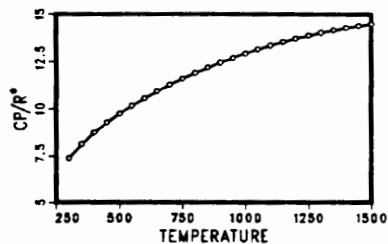
("ME" = CH<sub>3</sub>, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|-----------------|----------------|----------------|-----------------|
| 0300-0600K   | 0.01784749E+02 | 0.02058861E+00 | 0.03548509E-04 | -0.04111927E-06 | 0.03108978E-09 | 0.13184225E+05 | 0.01700701E+03  |
| 0600-1500K   | 0.05318279E+02 | 0.09490931E-01 | 0.02277164E-05 | -0.03005070E-07 | 0.09037830E-11 | 0.12535338E+05 | -0.10657105E+00 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \text{** } CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \text{** } H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \text{*** } S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HGAME2

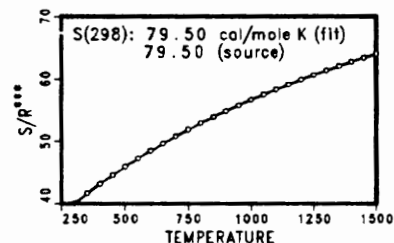
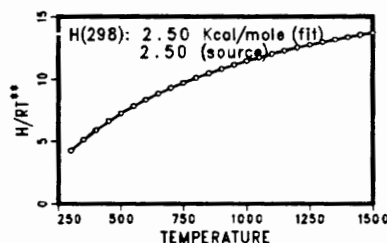
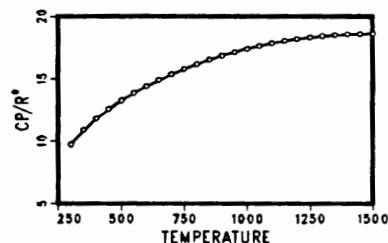
("ME" = CH<sub>3</sub>, METHYL)

GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | 0.09039155E+01 | 0.03264779E+00 | 0.05389243E-04  | -0.06814504E-06 | 0.05150323E-09 | -0.03978242E+04 | 0.02539304E+03  |
| 0600-1500K   | 0.06759397E+02 | 0.14261030E-01 | -0.11740239E-06 | -0.05001401E-07 | 0.15027851E-11 | -0.14732646E+04 | -0.02967135E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \text{** } CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \text{** } H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \text{*** } S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

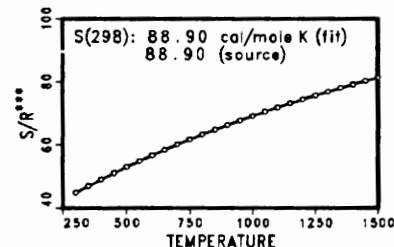
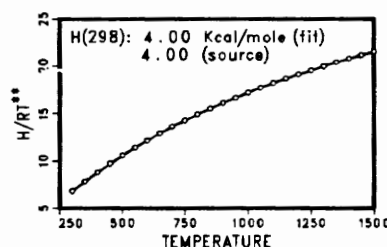
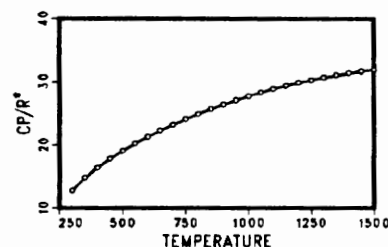
Species: HMEGAET

("ME"=CH<sub>3</sub>, METHYL; "ET"=C<sub>2</sub>H<sub>5</sub>, ETHYL) GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.02079142E+02 | 0.05373076E+00 | 0.11810364E-04 | -0.10998548E-06 | 0.08189554E-09 | 0.03216961E+04  | 0.04086070E+03  |
| 0600-1500K   | 0.07025463E+02  | 0.02564787E+00 | 0.09619100E-05 | -0.08403699E-07 | 0.02488860E-10 | -0.13613768E+04 | -0.03319484E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \text{** } CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \text{** } H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \text{*** } S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HN3

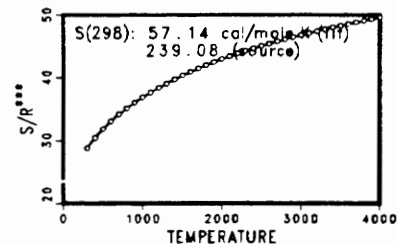
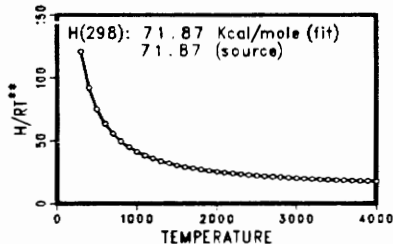
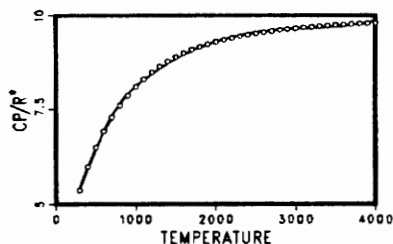
HYDRAZOIC ACID

GAS

As of: 8/26/87

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6             | a7              |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03621003E+02 | 0.06030785E-01 | 0.04054460E-05  | -0.02545270E-07 | 0.06174280E-11 | 0.03482373E+06 | 0.06333769E+02  |
| 1000-4000K   | 0.06023015E+02 | 0.02454362E-01 | -0.02404279E-05 | -0.13229726E-09 | 0.02474146E-12 | 0.03394051E+06 | -0.07015537E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: HNCO

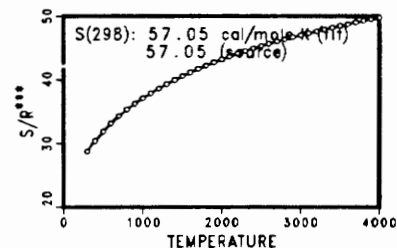
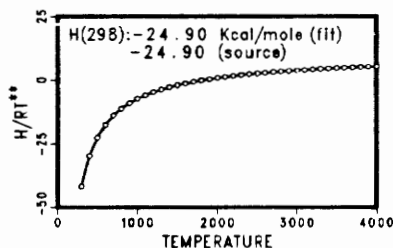
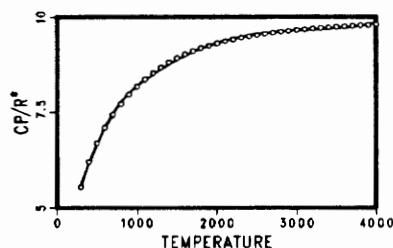
ISOCYANIC ACID

GAS

As of: 3/12/87

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6              | a7              |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.03694059E+02 | 0.06657236E-01 | -0.05054468E-06 | -0.03473411E-07 | 0.13605694E-11 | -0.13919758E+05 | 0.05712742E+02  |
| 1000-4000K   | 0.06211867E+02 | 0.02297137E-01 | -0.02216128E-05 | -0.12220438E-09 | 0.02272406E-12 | -0.14770725E+05 | -0.08016633E+02 |



Source: FIT TO BAC-MP4 DATA WITH H298=-24.9 PER MILLER

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: HNF

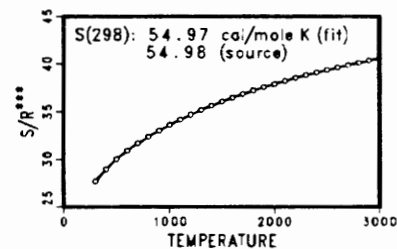
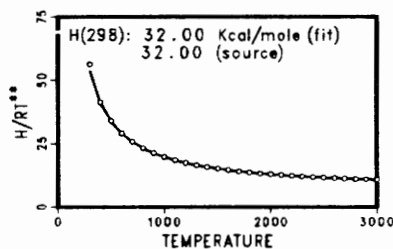
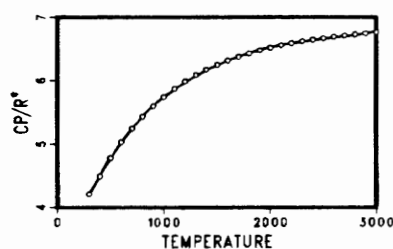
MONOFLUOROAMIDOGEN

GAS

As of: 4/24/89

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6             | a7             |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.03249760E+02 | 0.03261817E-01 | 0.04355642E-06  | -0.11002765E-08 | 0.02926757E-11 | 0.14991264E+05 | 0.08187434E+02 |
| 1000-3000K   | 0.04133219E+02 | 0.01912056E-01 | -0.16253301E-06 | -0.01726461E-08 | 0.03743691E-12 | 0.14670521E+05 | 0.03292122E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: HNF2

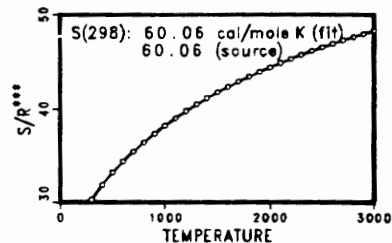
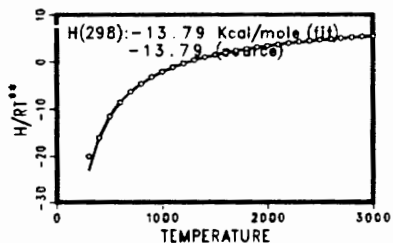
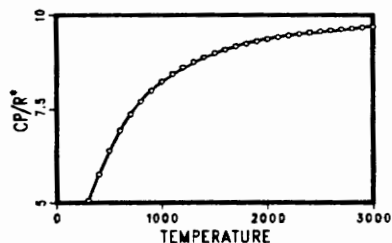
DIFLUOROAMMONIA

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.02572812E+02 | 0.08762144E-01 | -0.02326921E-05 | -0.05000826E-07 | 0.02143837E-10 | -0.08086760E+05 | 0.13006610E+02  |
| 1000-3000K   | 0.05704866E+02 | 0.03049897E-01 | -0.02826802E-05 | -0.02923184E-08 | 0.06551055E-12 | -0.09107488E+05 | -0.03941331E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HNO

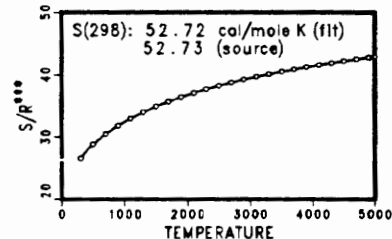
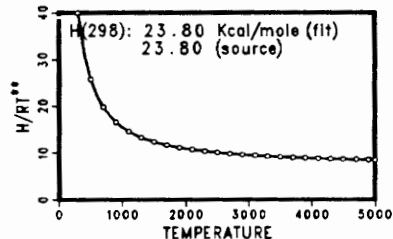
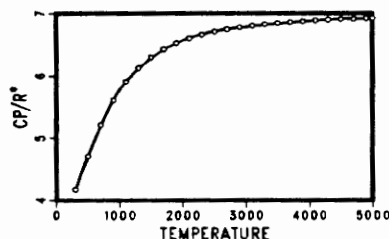
NITROXYL

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02784402E+02 | 0.06609646E-01 | -0.09300223E-04 | 0.09437980E-07 | -0.03753146E-10 | 0.10918779E+05 | 0.09035629E+02 |
| 1000-5000K   | 0.03615144E+02 | 0.03212485E-01 | -0.12603370E-05 | 0.02267297E-08 | -0.15362358E-13 | 0.10661911E+05 | 0.04810263E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HNO3

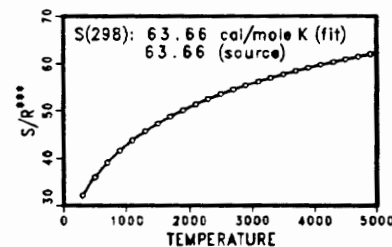
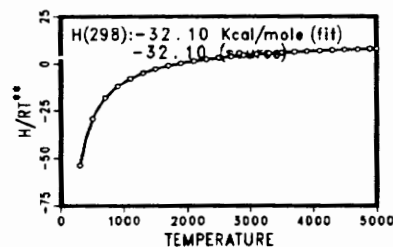
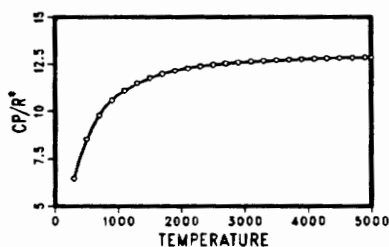
NITRIC ACID

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.13531850E+01 | 0.02220024E+00 | -0.01978811E-03 | 0.08773908E-07 | -0.16583844E-11 | -0.01738562E+06 | 0.01851868E+03  |
| 1000-5000K   | 0.07003844E+02 | 0.05811493E-01 | -0.02333788E-04 | 0.04288814E-08 | -0.02959385E-12 | -0.01889952E+06 | -0.10478628E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HO2

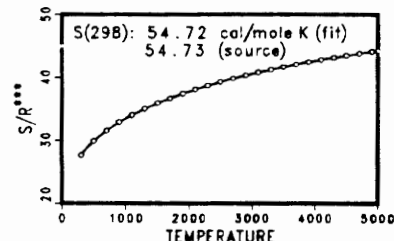
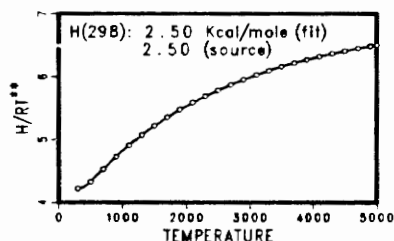
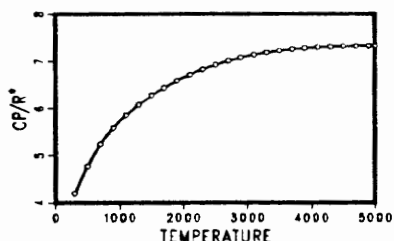
HYDROPEROXYL

GAS

As of: 2/03/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.02979963E+02 | 0.04996697E-01 | -0.03790997E-04 | 0.02354192E-07 | -0.08089024E-11 | 0.01762273E+04  | 0.09222724E+02 |
| 1000-5000K   | 0.04072191E+02 | 0.02131296E-01 | -0.05308145E-05 | 0.06112269E-09 | -0.02841164E-13 | -0.15797270E+03 | 0.03476029E+02 |



Source: SNLL FIT TO JANAF TABLES WITH H298=2.5 PER MILLER

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HOCN

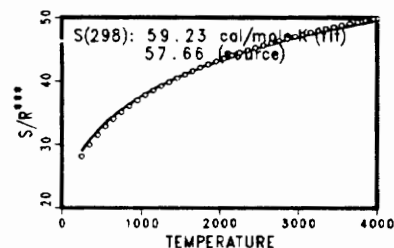
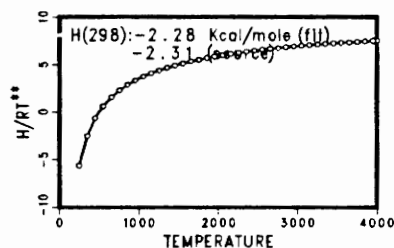
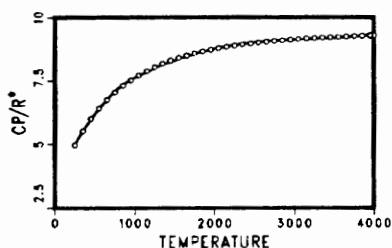
CYANIC ACID TRANS

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0250-1000K   | 0.03628292E+02 | 0.05664184E-01 | -0.11702056E-06 | -0.02348638E-07 | 0.08016402E-11 | -0.02475925E+05 | 0.07476825E+02  |
| 1000-4000K   | 0.05645607E+02 | 0.02298206E-01 | -0.02162629E-05 | -0.12148014E-09 | 0.02238636E-12 | -0.03178109E+05 | -0.03590263E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HONO

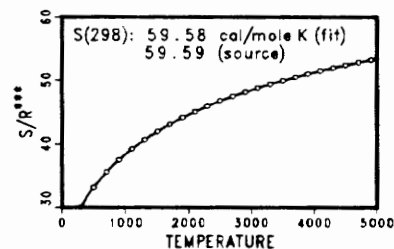
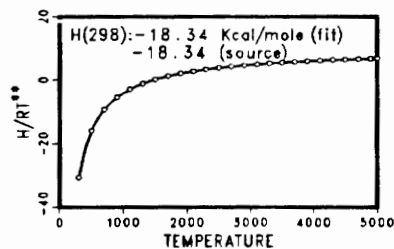
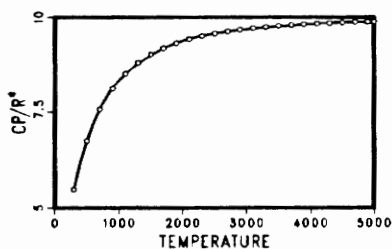
NITROUS ACID, CIS-

GAS

As of: 3/17/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02290413E+02 | 0.14099223E-01 | -0.13678717E-04 | 0.07498780E-07 | -0.01876905E-10 | -0.10431945E+05 | 0.13280769E+02  |
| 1000-5000K   | 0.05486892E+02 | 0.04218064E-01 | -0.16491426E-05 | 0.02971876E-08 | -0.02021148E-12 | -0.11268646E+05 | -0.02997002E+02 |



Source: SNLL FIT TO JANAF TABLES (HNO2)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HSI(NH2)2

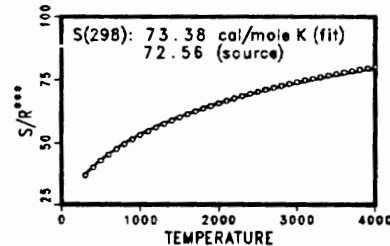
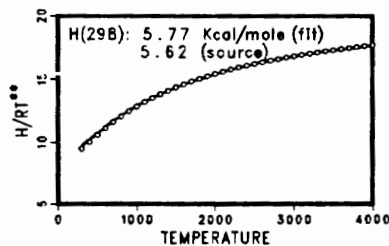
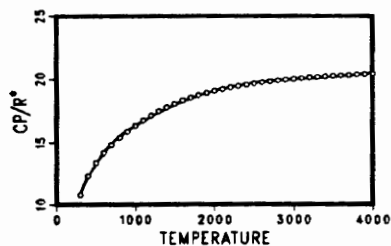
DIAMINOSILANE

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.06289698E+02 | 0.16750596E-01 | -0.15208775E-05 | -0.10700650E-07 | 0.05538640E-10 | 0.03154770E+04  | -0.03746008E+02 |
| 1000-4000K   | 0.11716773E+02 | 0.05339021E-01 | -0.04667823E-05 | -0.02824087E-08 | 0.05080915E-12 | -0.12641686E+04 | -0.03245117E+03 |



Source: SNL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HSI(NH2)3

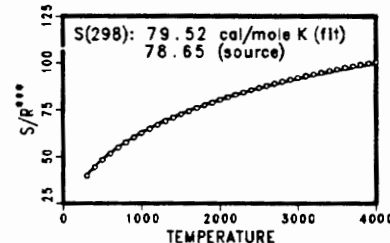
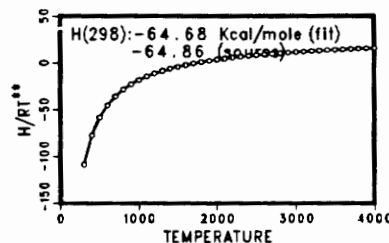
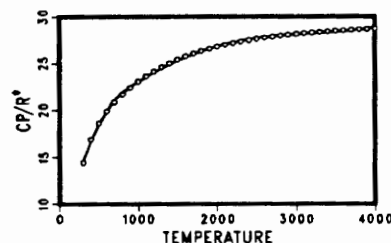
TRIAMINOSILANE

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.07070983E+02 | 0.02754435E+00 | -0.02603669E-04 | -0.01874567E-06 | 0.09778511E-10 | -0.03582658E+06 | -0.08209675E+02 |
| 1000-4000K   | 0.16614058E+02 | 0.07395874E-01 | -0.06440009E-05 | -0.03918887E-08 | 0.07045959E-12 | -0.03859547E+06 | -0.05865317E+03 |



Source: SNL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HSiCl

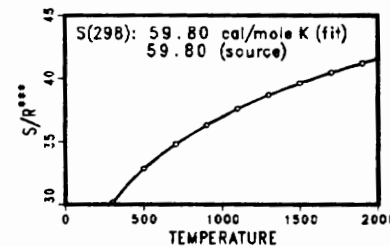
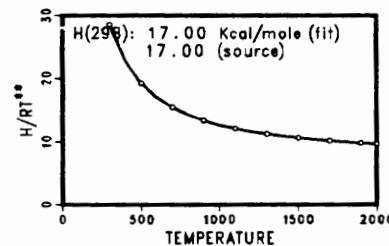
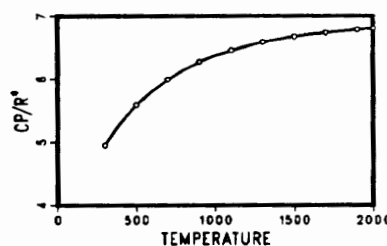
CHLOROSILYLENE

GAS

As of: 12/19/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03072747E+02 | 0.09057843E-01 | -0.11591338E-04 | 0.08310476E-07  | -0.02482999E-10 | 0.07324210E+05 | 0.10334904E+02 |
| 1000-2000K   | 0.04900627E+02 | 0.01981752E-01 | -0.03634646E-05 | -0.02285211E-08 | 0.07633527E-12  | 0.06914634E+05 | 0.13770041E+01 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HSIN

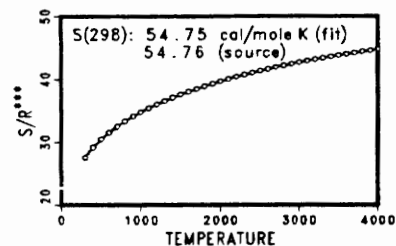
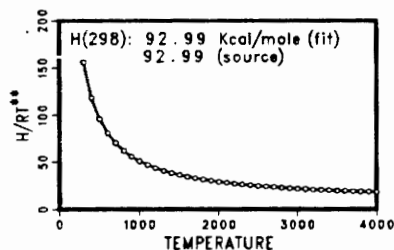
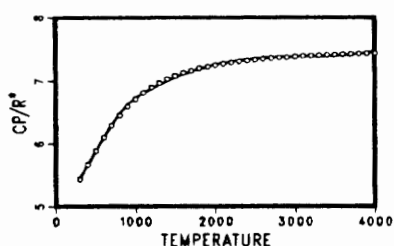
SILANITRILE

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04865176E+02 | 0.01775119E-01 | 0.04890869E-05  | 0.03922382E-08  | -0.07913276E-11 | 0.04526352E+06 | -0.07134509E+01 |
| 1000-4000K   | 0.05746590E+02 | 0.11671186E-02 | -0.13607424E-06 | -0.05908616E-09 | 0.11746961E-13  | 0.04484671E+06 | -0.05931788E+02 |



Source: SNL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

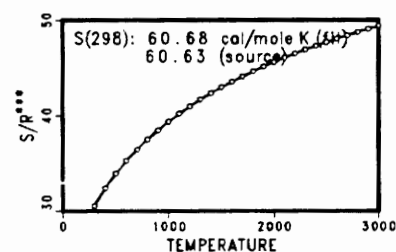
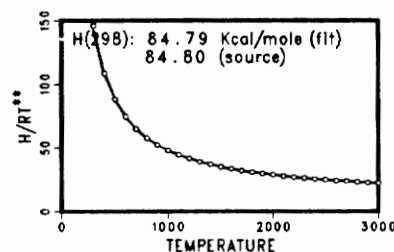
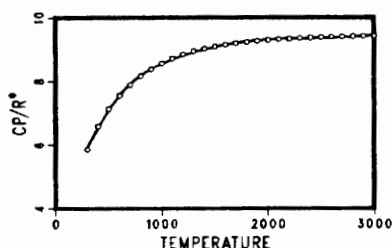
Species: HSINH

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03566343E+02 | 0.08446736E-01 | -0.07699952E-05 | -0.05270970E-07 | 0.02581065E-10 | 0.04124903E+06 | 0.07780791E+02  |
| 1000-3000K   | 0.06493435E+02 | 0.02567980E-01 | -0.03126526E-05 | -0.02577467E-08 | 0.06216479E-12 | 0.04035934E+06 | -0.07830112E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HSINH2

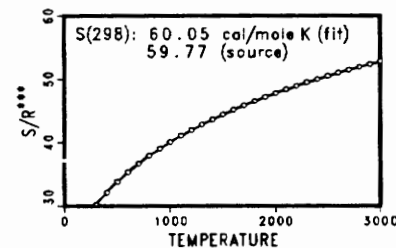
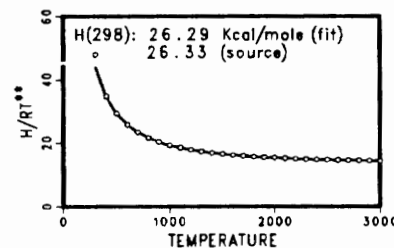
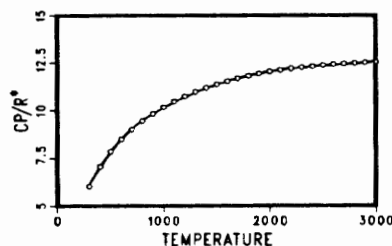
AMINOSILYLENE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02716144E+02 | 0.12042781E-01 | -0.09827195E-05 | -0.07408477E-07 | 0.03789792E-10 | 0.11907715E+05 | 0.11262523E+02  |
| 1000-3000K   | 0.06177894E+02 | 0.04689964E-01 | -0.03583293E-05 | -0.04457980E-08 | 0.09379187E-12 | 0.10912773E+05 | -0.07006672E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: I\*C3H7

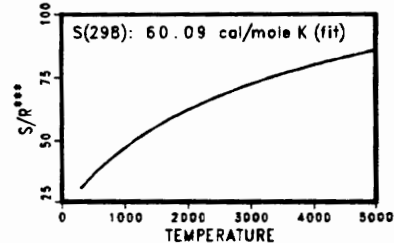
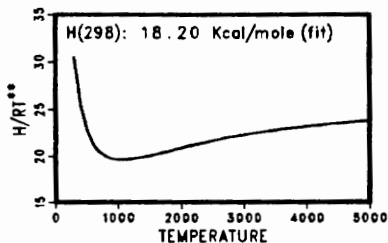
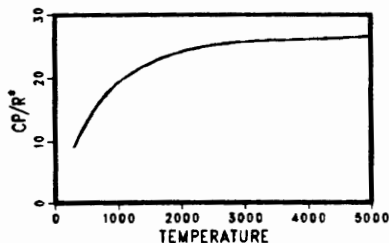
ISOPROPYL RAD

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.01713299E+02 | 0.02542616E+00 | 0.15808083E-05  | -0.01821286E-06 | 0.08827710E-10  | 0.07535808E+05 | 0.12979008E+02  |
| 1000-5000K   | 0.08063369E+02 | 0.15744876E-01 | -0.05182391E-04 | 0.07477245E-08  | -0.03854422E-12 | 0.05313871E+05 | -0.02192646E+03 |



Source: BURCAT (TECHNION REPORTS)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

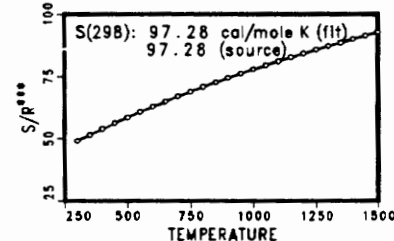
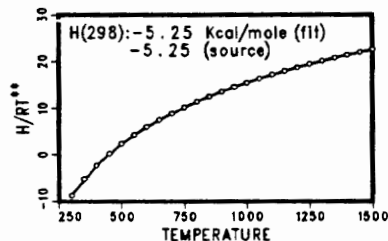
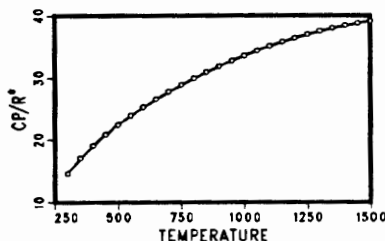
Species: ME2GAET

("ME"=CH3,METHYL; "ET"=C2H5,ETHYL) GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.03218207E+02 | 0.06398884E+00 | 0.15545521E-04 | -0.12847095E-06 | 0.09441259E-09 | -0.04451897E+05 | 0.04848091E+03  |
| 0600-1500K   | 0.07174541E+02  | 0.03235532E+00 | 0.14951986E-05 | -0.10482260E-07 | 0.03053961E-10 | -0.06383914E+05 | -0.02026765E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

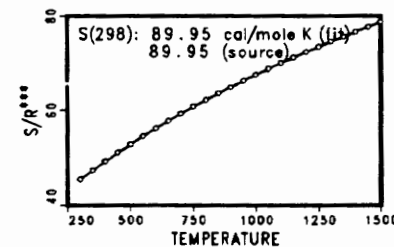
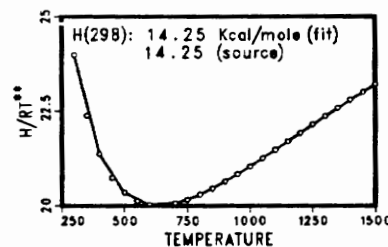
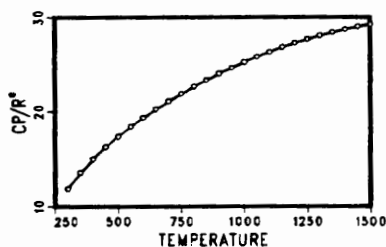
Species: MEGAET

("ME"=CH3,METHYL; "ET"=C2H5,ETHYL) GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|-----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-0600K   | -0.08169937E+01 | 0.04554296E+00 | 0.10531326E-04 | -0.09079987E-06 | 0.06700563E-09 | 0.05448005E+05 | 0.03655501E+03 |
| 0600-1500K   | 0.06600990E+02  | 0.02284791E+00 | 0.10133754E-05 | -0.07318045E-07 | 0.02140196E-10 | 0.04071592E+05 | 0.05239051E+01 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



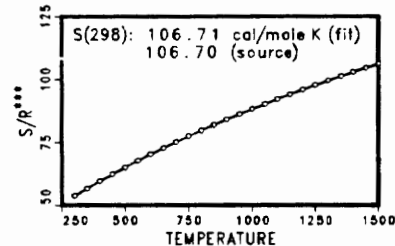
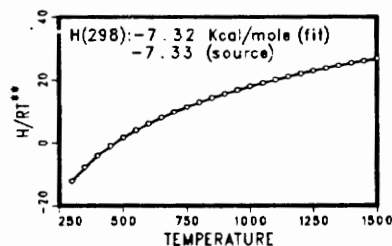
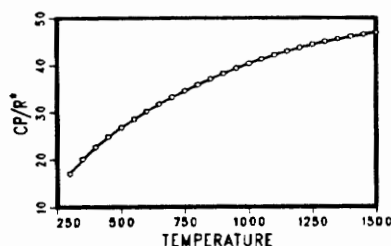
Species: MEGAET2

("ME"=CH3,METHYL; "ET"=C2H5,ETHYL) GAS

As of: 6/29/87

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0300-0600K   | -0.05607498E+02 | 0.08187357E+00 | 0.01920530E-03 | -0.01678978E-05 | 0.12433538E-09 | -0.05546687E+05 | 0.06163371E+03  |
| 0600-1500K   | 0.08123155E+02  | 0.03978908E+00 | 0.01690979E-04 | -0.13084149E-07 | 0.03852598E-10 | -0.08091056E+05 | -0.05039992E+02 |



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: N

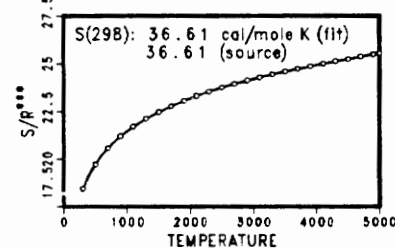
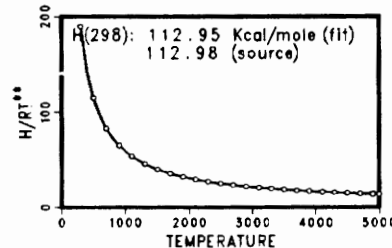
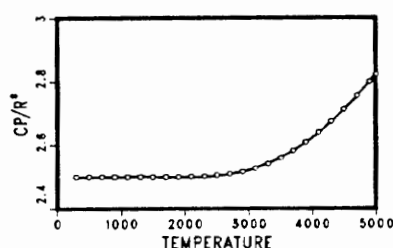
NITROGEN, MONATOMIC

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02503071E+02 | -0.02180018E-03 | 0.05420529E-06  | -0.05647560E-09 | 0.02099904E-12  | 0.05609890E+06 | 0.04167566E+02 |
| 1000-5000K   | 0.02450268E+02 | 0.10661458E-03  | -0.07465337E-06 | 0.01879652E-09  | -0.10259839E-14 | 0.05611604E+06 | 0.04448758E+02 |



Source: NASA FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: N\*C3H7

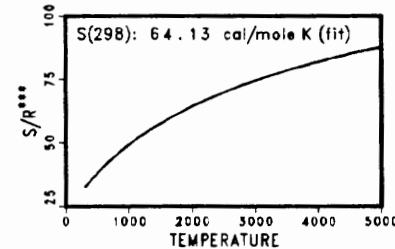
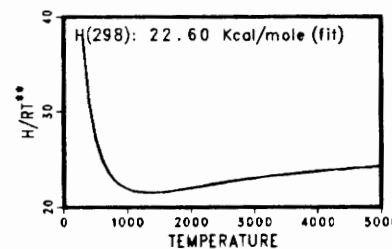
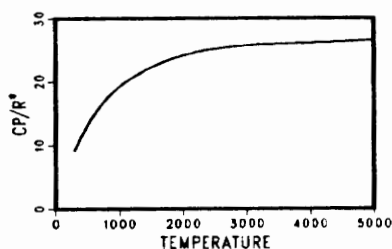
N-PROPYL RAD

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.01922536E+02 | 0.02478927E+00 | 0.01810249E-04  | -0.01783265E-06 | 0.08582996E-10  | 0.09713281E+05 | 0.13992715E+02  |
| 1000-5000K   | 0.07978290E+02 | 0.15761134E-01 | -0.05173243E-04 | 0.07443892E-08  | -0.03824978E-12 | 0.07579402E+05 | -0.01935611E+03 |



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: N2

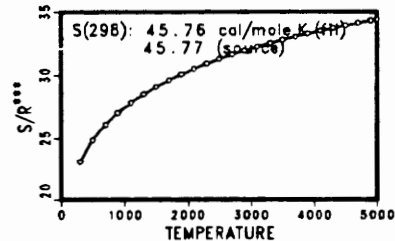
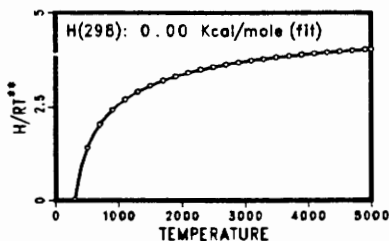
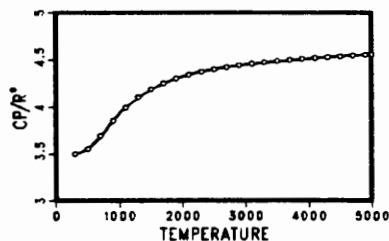
NITROGEN, DIATOMIC (REF ST)

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03298677E+02 | 0.14082404E-02 | -0.03963222E-04 | 0.05641515E-07 | -0.02444854E-10 | -0.10208999E+04 | 0.03950372E+02 |
| 1000-5000K   | 0.02926640E+02 | 0.14879768E-02 | -0.05684760E-05 | 0.10097038E-09 | -0.06753351E-13 | -0.09227977E+04 | 0.05980528E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: N2H2

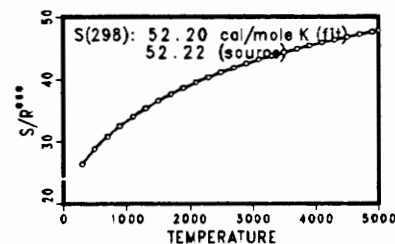
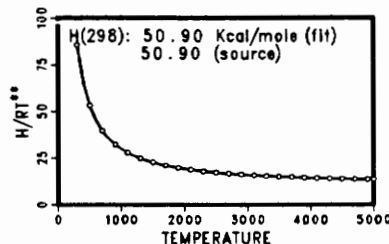
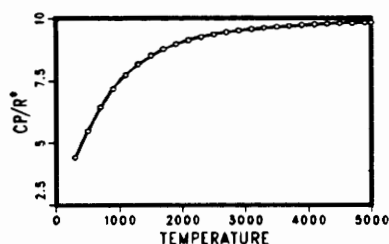
DI-IMIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.16179994E+01 | 0.13063122E-01 | -0.01715711E-03 | 0.16056079E-07 | -0.06093638E-10 | 0.02467526E+06 | 0.13794670E+02 |
| 1000-5000K   | 0.03371185E+02 | 0.06039968E-01 | -0.02303853E-04 | 0.04062789E-08 | -0.02713144E-12 | 0.02418172E+06 | 0.04980585E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

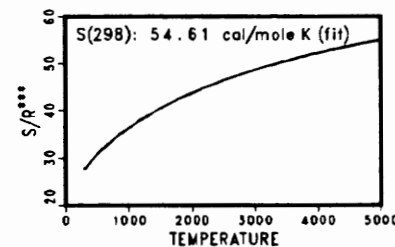
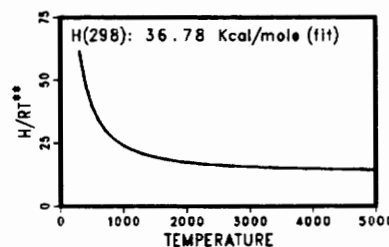
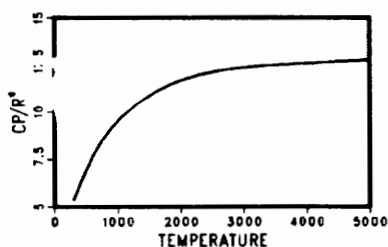
Species: N2H3

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03174203E+02 | 0.04715907E-01 | 0.13348671E-04  | -0.01919684E-06 | 0.07487563E-10  | 0.01727269E+06 | 0.07557224E+02  |
| 1000-5000K   | 0.04441846E+02 | 0.07214270E-01 | -0.02495684E-04 | 0.03920564E-08  | -0.02298949E-12 | 0.16642211E+05 | -0.04275204E+01 |



Source: SNLL FIT TO BAHN DATA OF 1973

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: N2H4

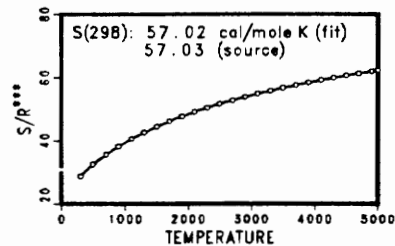
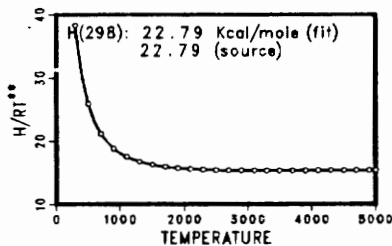
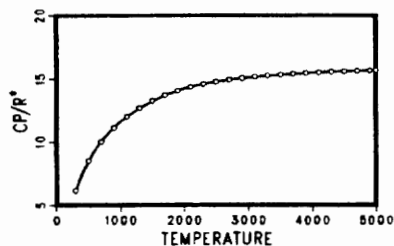
HYDRAZINE

GAS

As of: 12/12/86

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K | 0.06442605E+00 | 0.02749729E+00 | -0.02899451E-03 | 0.01745239E-06 | -0.04422282E-10 | 0.10451917E+05 | 0.02127789E+03  |
| 1000-5000K | 0.04977317E+02 | 0.09595519E-01 | -0.03547639E-04 | 0.06124299E-08 | -0.04029795E-12 | 0.09341219E+05 | -0.02962989E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: N2H4(L)

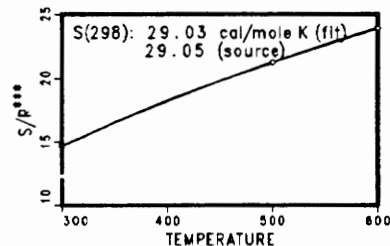
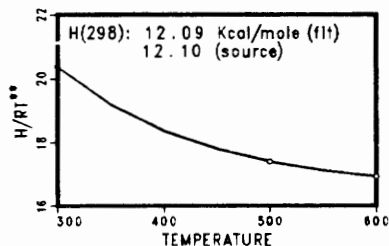
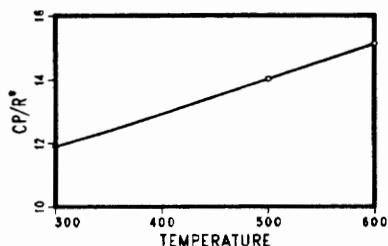
HYDRAZINE

LIQUID

As of: 9/05/89

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|------------|----------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|
| 0300-0450K | 0.09047444E+02 | 0.09241592E-01 | 0.02263547E-04 | -0.08952247E-07 | 0.14868629E-10  | 0.02970392E+05 | -0.03974033E+03 |
| 0450-0600K | 0.08890683E+02 | 0.08330343E-01 | 0.04945549E-04 | -0.04909251E-08 | -0.03355824E-10 | 0.03032250E+05 | -0.03871433E+03 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: N2O

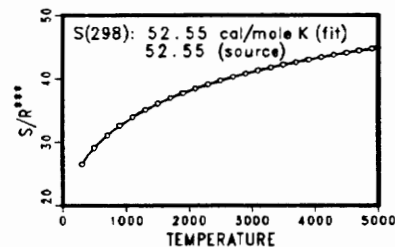
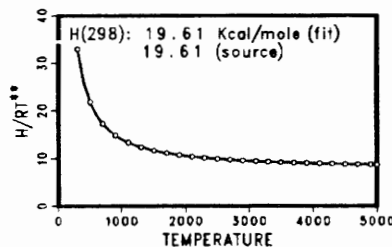
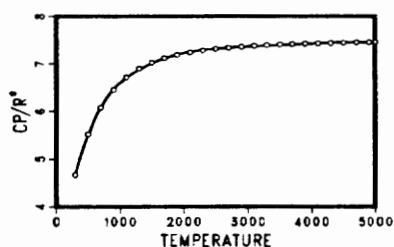
DINITROGEN MONOXIDE

GAS

As of: 12/12/86

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K | 0.02543057E+02 | 0.09492193E-01 | -0.09792775E-04 | 0.06263844E-07 | -0.01901825E-10 | 0.08765100E+05 | 0.09511222E+02  |
| 1000-5000K | 0.04718977E+02 | 0.02873713E-01 | -0.11974958E-05 | 0.02250551E-08 | -0.15753370E-13 | 0.08165811E+05 | -0.16572504E+01 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

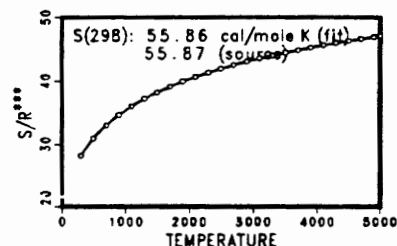
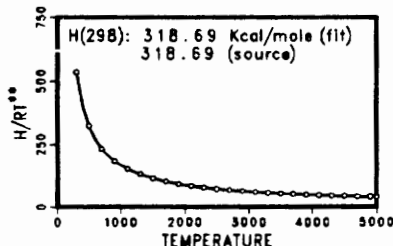
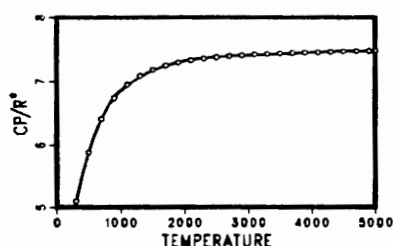
Species: N2O+

DINITROGEN MONOXIDE, UNIPOSITIVE ION GAS

As of: 12/12/86

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K | 0.03187228E+02 | 0.08350714E-01 | -0.07894548E-04 | 0.04597444E-07 | -0.13810748E-11 | 0.15912794E+06 | 0.07779425E+02  |
| 1000-5000K | 0.05398516E+02 | 0.02249478E-01 | -0.09577056E-05 | 0.01823192E-08 | -0.12844222E-13 | 0.15848513E+06 | -0.03733146E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: N2O4

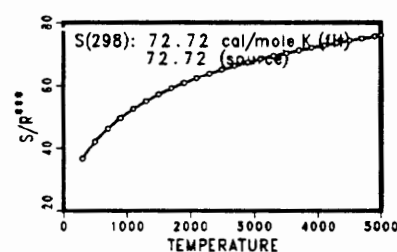
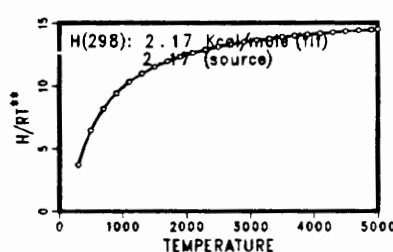
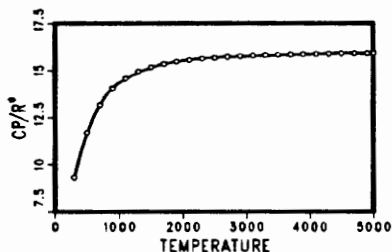
NITROGEN TETROXIDE

GAS

As of: 12/12/86

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K | 0.03624592E+02 | 0.02474708E+00 | -0.02172874E-03 | 0.09927103E-07 | -0.02222817E-10 | -0.09128241E+04 | 0.09457174E+02  |
| 1000-5000K | 0.10482201E+02 | 0.05972272E-01 | -0.02564043E-04 | 0.04916885E-08 | -0.03490969E-12 | -0.02849988E+05 | -0.02612289E+03 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: N3

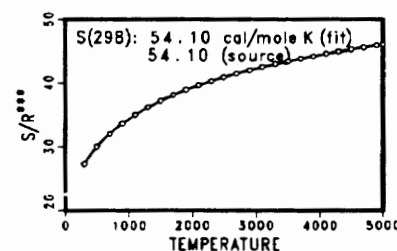
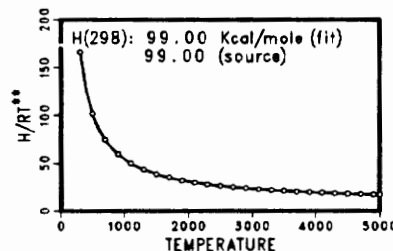
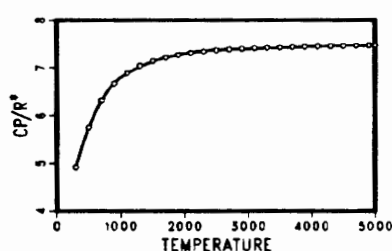
AZIDE

GAS

As of: 12/12/86

Fit  
Coefficients

|            | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K | 0.02882218E+02 | 0.08930338E-01 | -0.08539038E-04 | 0.05045585E-07 | -0.15212480E-11 | 0.04863468E+06 | 0.08481757E+02  |
| 1000-5000K | 0.05208505E+02 | 0.02444507E-01 | -0.10389415E-05 | 0.01977416E-08 | -0.13956436E-13 | 0.04796178E+06 | -0.03612755E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NCO

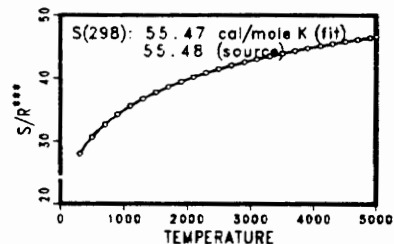
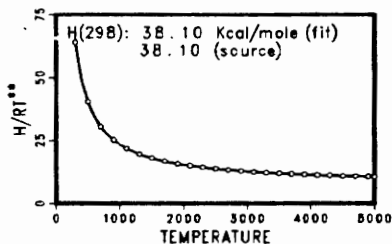
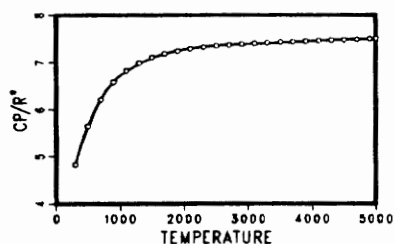
NCO RADICAL

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02830320E+02 | 0.08871490E-01 | -0.08945636E-04 | 0.05876918E-07 | -0.01907734E-10 | 0.01800543E+06 | 0.09498831E+02  |
| 1000-5000K   | 0.05012045E+02 | 0.02626773E-01 | -0.11082433E-05 | 0.02093860E-08 | -0.14603470E-13 | 0.01737185E+06 | -0.01830075E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NF

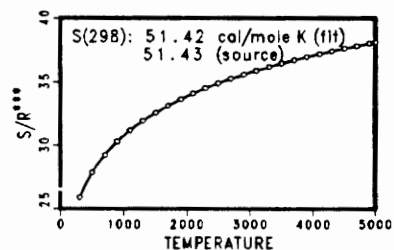
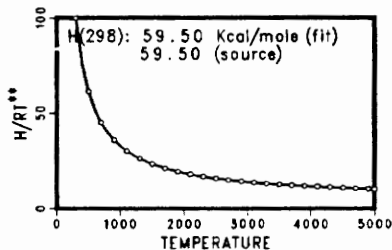
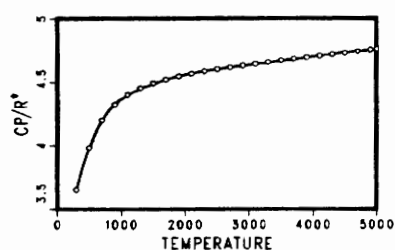
NITROGEN MONOFLUORIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02871947E+02 | 0.03312192E-01 | -0.02691158E-04 | 0.11219514E-08 | -0.02475130E-11 | 0.02896257E+06 | 0.08640247E+02 |
| 1000-5000K   | 0.03862176E+02 | 0.07551806E-02 | -0.03044942E-05 | 0.05874447E-09 | -0.04187479E-13 | 0.02867242E+06 | 0.03457232E+02 |



Source: SNLL FIT TO JANAF TABLES (FN)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NFO

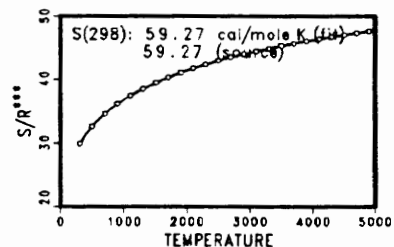
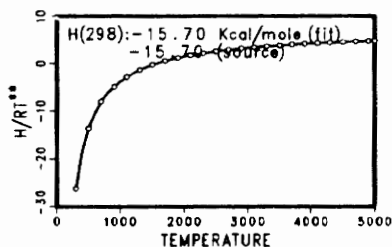
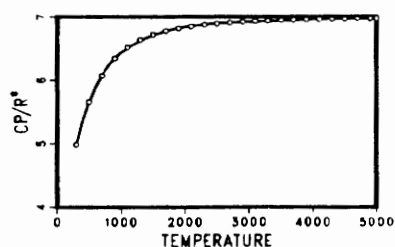
NITROSYL FLUORIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.03352307E+02 | 0.07229966E-01 | -0.06951136E-04 | 0.03828526E-07 | -0.10235582E-11 | -0.09167035E+05 | 0.08854189E+02  |
| 1000-5000K   | 0.05174520E+02 | 0.01938472E-01 | -0.08222701E-05 | 0.15642909E-09 | -0.11044974E-13 | -0.09670935E+05 | -0.05352460E+01 |



Source: SNLL FIT TO JANAF TABLES (FNO)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NF02

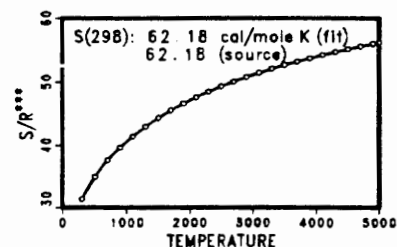
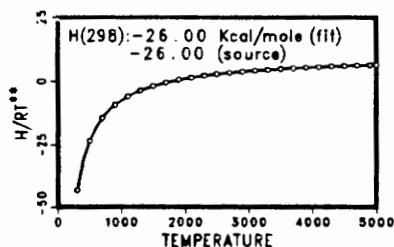
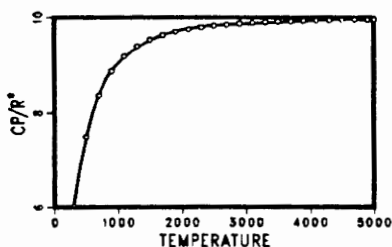
NITRYL FLUORIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02447528E+02 | 0.15441095E-01 | -0.13005952E-04 | 0.04856383E-07 | -0.06852266E-11 | -0.14393999E+05 | 0.13283604E+02  |
| 1000-5000K   | 0.06816857E+02 | 0.03462639E-01 | -0.14922156E-05 | 0.02869665E-08 | -0.02041856E-12 | -0.15602619E+05 | -0.09320129E+02 |



Source: SNLL FIT TO JANAF TABLES (FN02)

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NH

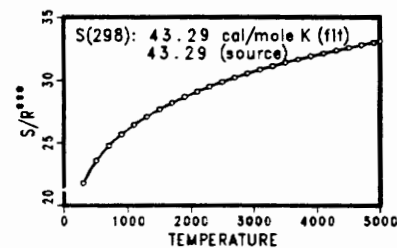
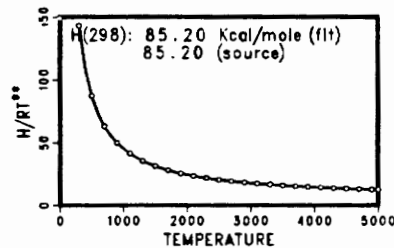
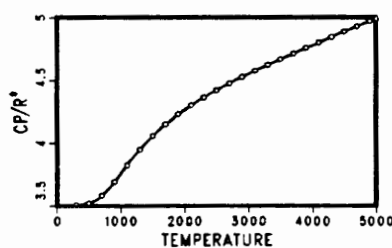
IMIDOGEN

GAS

As of: 3/13/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03339758E+02 | 0.12530086E-02 | -0.03491645E-04 | 0.04218812E-07 | -0.15576179E-11 | 0.04185047E+06 | 0.02507180E+02 |
| 1000-5000K   | 0.02760249E+02 | 0.13753463E-02 | -0.04451914E-05 | 0.07692791E-09 | -0.05017592E-13 | 0.04207828E+06 | 0.05857199E+02 |



Source: FIT JANAF TABLES WITH H298=85.2 PER MILLER

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NH2

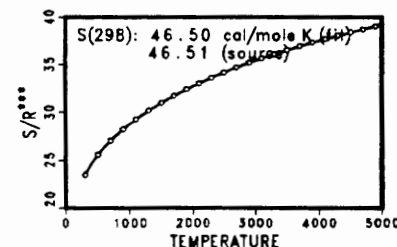
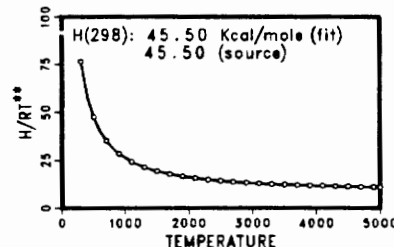
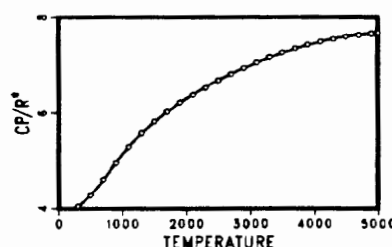
AMIDOGEN

GAS

As of: 12/16/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03432493E+02 | 0.03299540E-01 | -0.06613600E-04 | 0.08590947E-07 | -0.03572046E-10 | 0.02177227E+06 | 0.03090110E+02 |
| 1000-5000K   | 0.02961311E+02 | 0.02932699E-01 | -0.09063600E-05 | 0.16172575E-09 | -0.12042003E-13 | 0.02191976E+06 | 0.05777878E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NH3

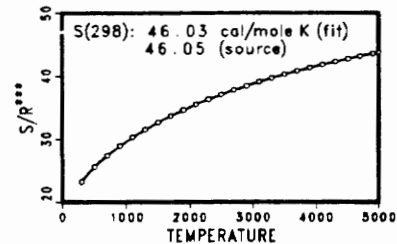
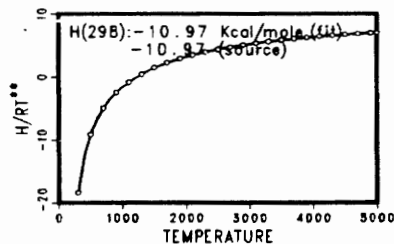
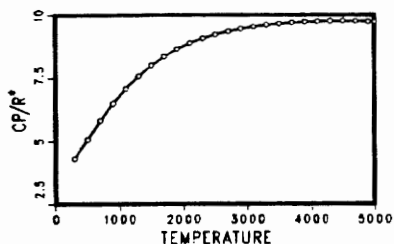
AMMONIA

GAS

As of: 12/13/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.02204351E+02 | 0.10114765E-01 | -0.14652648E-04 | 0.14472350E-07 | -0.05328509E-10 | -0.06525488E+05 | 0.08127138E+02 |
| 1000-5000K   | 0.02461904E+02 | 0.06059166E-01 | -0.02004976E-04 | 0.03136003E-08 | -0.01938317E-12 | -0.06493269E+05 | 0.07472097E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

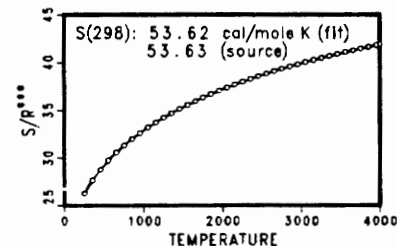
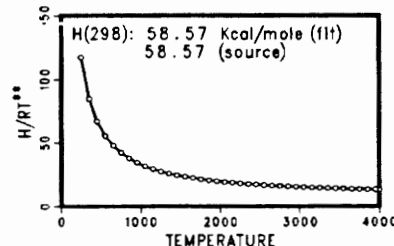
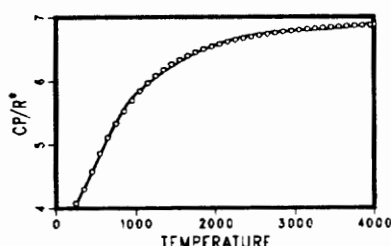
Species: NNH

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0250-1000K   | 0.03501344E+02 | 0.02053586E-01 | 0.07170409E-05  | 0.04921348E-08  | -0.09671170E-11 | 0.02833347E+06 | 0.06391837E+02 |
| 1000-4000K   | 0.04415342E+02 | 0.16143879E-02 | -0.16328943E-06 | -0.08559846E-09 | 0.16147909E-13  | 0.02788029E+06 | 0.09042888E+01 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NO

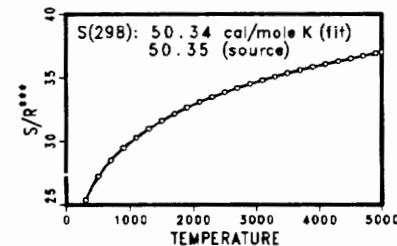
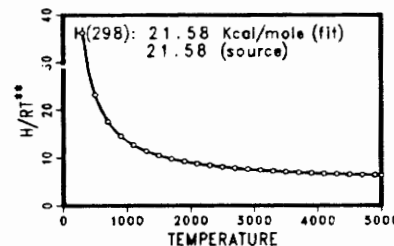
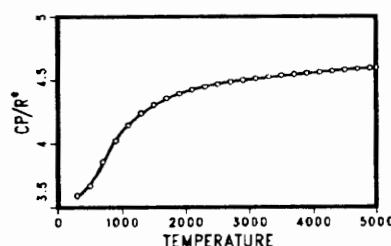
NITRIC OXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03376541E+02 | 0.12530634E-02 | -0.03302750E-04 | 0.05217810E-07 | -0.02446262E-10 | 0.09817961E+05 | 0.05829590E+02 |
| 1000-5000K   | 0.03245435E+02 | 0.12691383E-02 | -0.05015890E-05 | 0.09169283E-09 | -0.06275419E-13 | 0.09800840E+05 | 0.06417293E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NO+

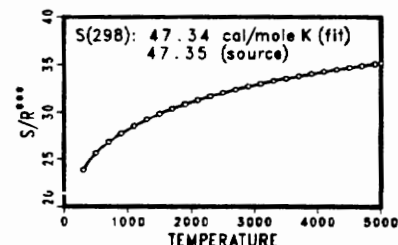
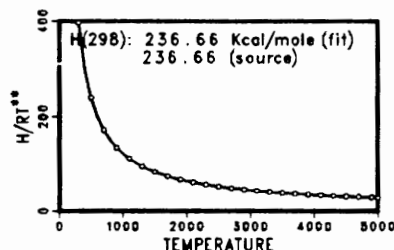
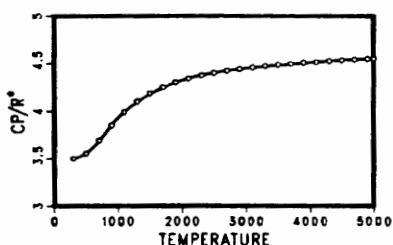
NITRIC OXIDE, UNIPosITIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03297349E+02 | 0.14228899E-02 | -0.04007441E-04 | 0.05670551E-07 | -0.02446971E-10 | 0.11808338E+06 | 0.04749948E+02 |
| 1000-5000K   | 0.02914888E+02 | 0.14993349E-02 | -0.05727972E-05 | 0.10177767E-09 | -0.06825390E-13 | 0.11818688E+06 | 0.06844346E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NO2

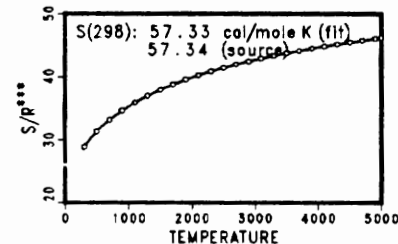
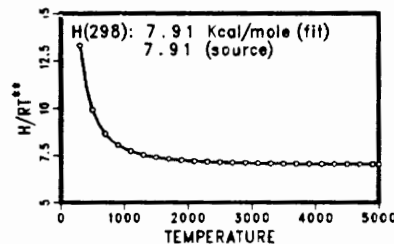
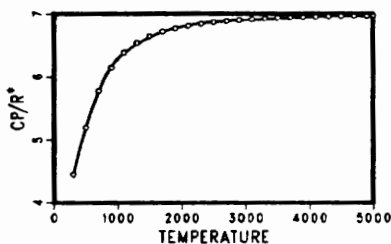
NITROGEN DIOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02670600E+02 | 0.07838500E-01 | -0.08063864E-04 | 0.06161714E-07 | -0.02320150E-10 | 0.02896290E+05 | 0.11612071E+02 |
| 1000-5000K   | 0.04682859E+02 | 0.02462429E-01 | -0.10422585E-05 | 0.01976902E-08 | -0.13917168E-13 | 0.02261292E+05 | 0.09885985E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: NO2-

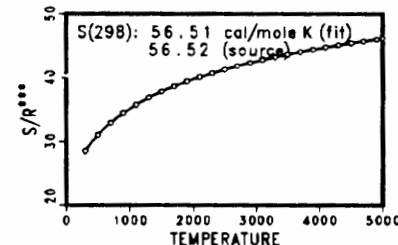
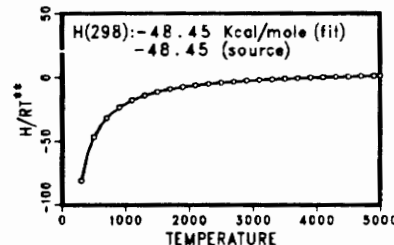
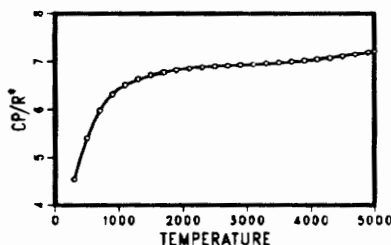
NITROGEN DIOXIDE, UNINEGATIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02448586E+02 | 0.08982507E-01 | -0.07853431E-04 | 0.03927276E-07 | -0.10716939E-11 | -0.02545097E+06 | 0.12130600E+02  |
| 1000-5000K   | 0.05043114E+02 | 0.02166427E-01 | -0.09455454E-05 | 0.01816313E-08 | -0.12383945E-13 | -0.02621553E+06 | -0.14459051E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



Species: NO3

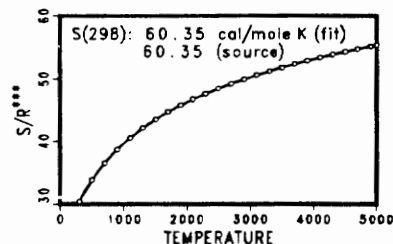
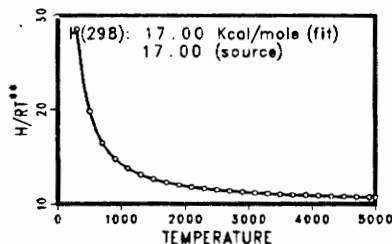
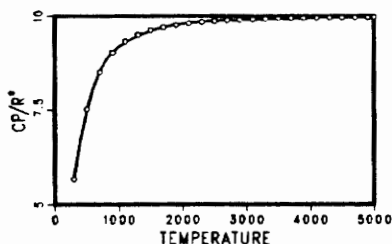
NITROGEN TRIOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.12210763E+01 | 0.01878797E+00 | -0.13443212E-04 | 0.12746013E-08 | 0.13540601E-11  | 0.07473144E+05 | 0.01840202E+03  |
| 1000-5000K   | 0.07120307E+02 | 0.03246228E-01 | -0.14316134E-05 | 0.02797053E-08 | -0.02013007E-12 | 0.05864479E+05 | -0.12137301E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: O

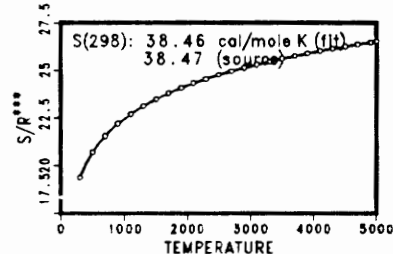
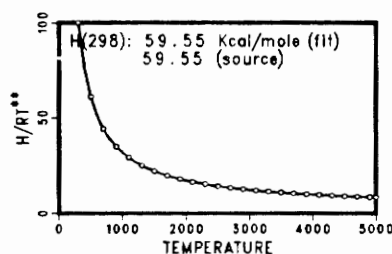
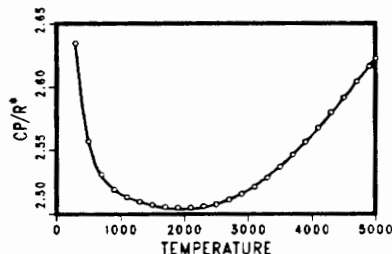
OXYGEN, MONATOMIC

GAS

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02946428E+02 | -0.16381665E-02 | 0.02421031E-04  | -0.16028431E-08 | 0.03890696E-11  | 0.02914764E+06 | 0.02963995E+02 |
| 1000-5000K   | 0.02542059E+02 | -0.02755061E-03 | -0.03102803E-07 | 0.04551067E-10  | -0.04368051E-14 | 0.02923080E+06 | 0.04920308E+02 |



Source: NASA FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: O+

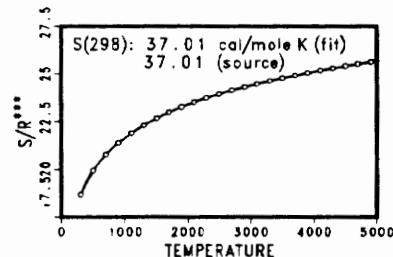
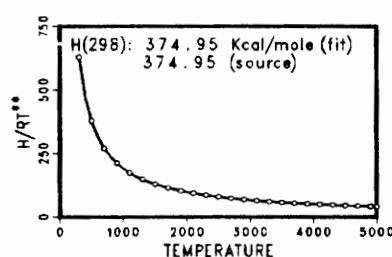
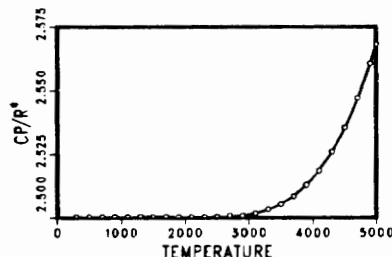
OXYGEN, UNIPOSITIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02499272E+02 | 0.05820598E-04  | -0.11209219E-07 | 0.08232108E-10  | -0.01916378E-13 | 0.01879556E+07 | 0.04384825E+02 |
| 1000-5000K   | 0.02501869E+02 | -0.06107262E-04 | 0.07324307E-07  | -0.03438353E-10 | 0.05506407E-14  | 0.01879552E+07 | 0.04372826E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: O-

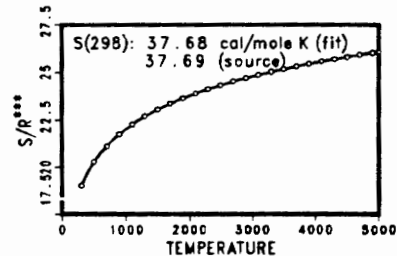
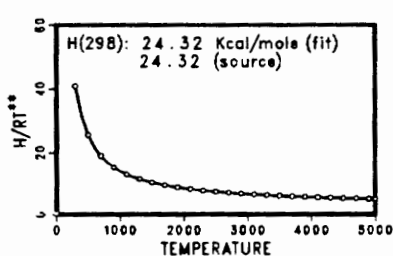
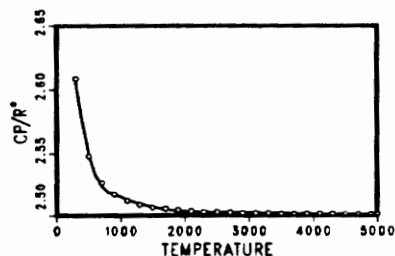
OXYGEN, UNINEGATIVE ION

GAS

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02747263E+02 | -0.05724860E-02 | 0.02712548E-05 | 0.02691511E-08  | -0.02002357E-11 | 0.11443947E+05 | 0.03469852E+02 |
| 1000-5000K   | 0.02559580E+02 | -0.07147887E-03 | 0.03301804E-06 | -0.06660944E-10 | 0.04900726E-14  | 0.11489346E+05 | 0.04426186E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: O2

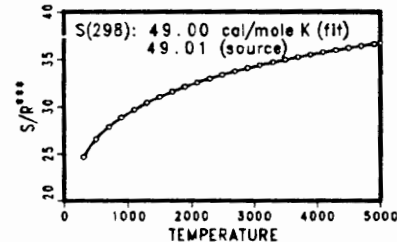
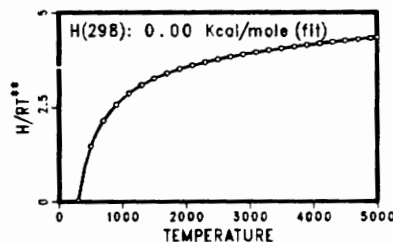
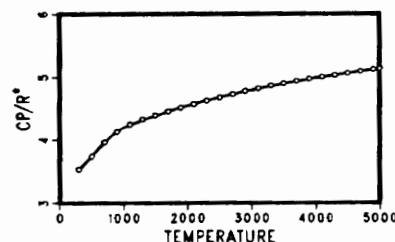
OXYGEN, DIATOMIC (REF ST)

GAS

As of: 12/13/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03212936E+02 | 0.11274864E-02 | -0.05756150E-05 | 0.13138773E-08 | -0.08768554E-11 | -0.10052490E+04 | 0.06034737E+02 |
| 1000-5000K   | 0.03697578E+02 | 0.06135197E-02 | -0.12588420E-06 | 0.01775281E-09 | -0.11364354E-14 | -0.12339301E+04 | 0.03189165E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: O2-

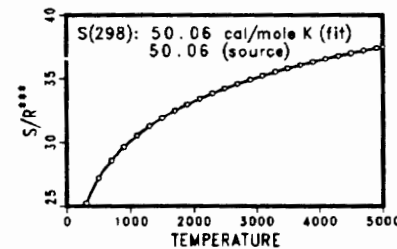
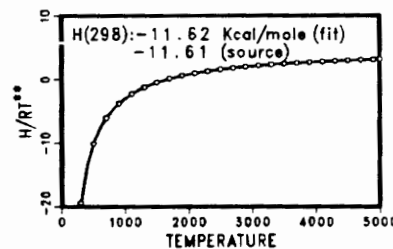
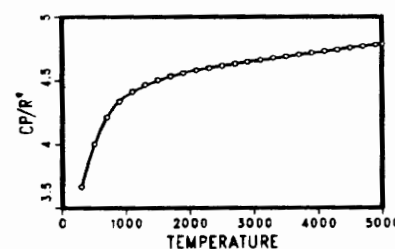
OXYGEN, DIATOMIC, UNINEGATIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.02872291E+02 | 0.03359716E-01 | -0.02664886E-04 | 0.09807524E-08 | -0.16709571E-12 | -0.06829094E+05 | 0.07938372E+02 |
| 1000-5000K   | 0.03883013E+02 | 0.07407872E-02 | -0.02961776E-05 | 0.05724304E-09 | -0.04086547E-13 | -0.07121644E+05 | 0.02658211E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: O3

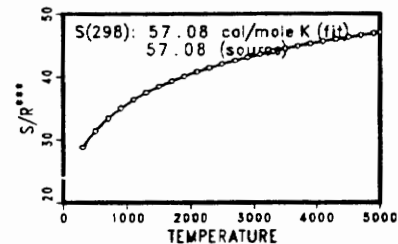
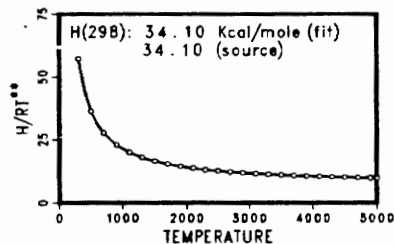
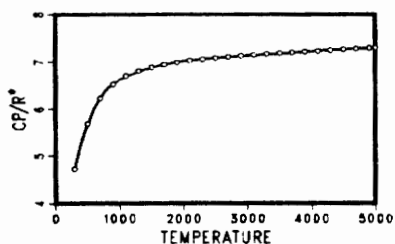
OZONE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02462608E+02 | 0.09582781E-01 | -0.07087359E-04 | 0.13633683E-08 | 0.02969647E-11  | 0.16061522E+05 | 0.12141870E+02  |
| 1000-5000K   | 0.05429371E+02 | 0.01820380E-01 | -0.07705607E-05 | 0.14992929E-09 | -0.10755629E-13 | 0.15235267E+05 | -0.03266386E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: OH

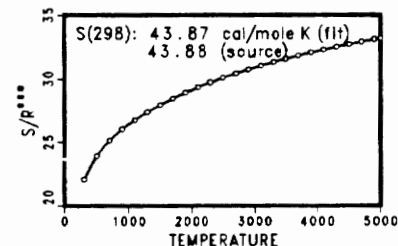
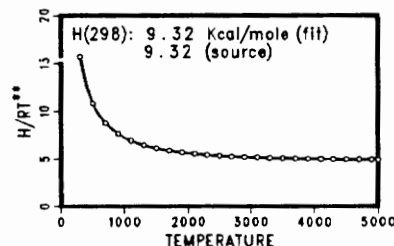
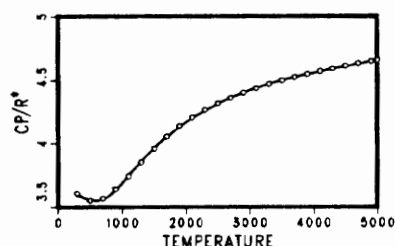
HYDROXYL

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03637266E+02 | 0.01850910E-02 | -0.16761646E-05 | 0.02387202E-07 | -0.08431442E-11 | 0.03606781E+05 | 0.13588605E+01 |
| 1000-5000K   | 0.02882730E+02 | 0.10139743E-02 | -0.02276877E-05 | 0.02174683E-09 | -0.05126305E-14 | 0.03886888E+05 | 0.05595712E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: OH+

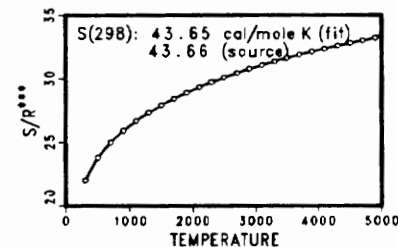
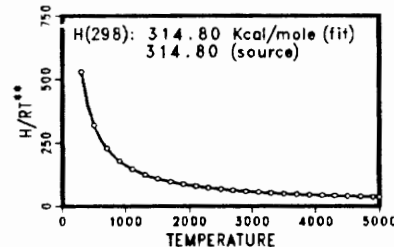
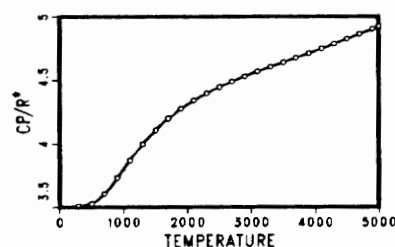
HYDROXYL, UNIPosITIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03326978E+02 | 0.13457859E-02 | -0.03777167E-04 | 0.04687749E-07 | -0.01780982E-10 | 0.15740294E+06 | 0.02744042E+02 |
| 1000-5000K   | 0.02719058E+02 | 0.15085714E-02 | -0.05029369E-05 | 0.08261951E-09 | -0.04947452E-13 | 0.15763414E+06 | 0.06234536E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: OH-

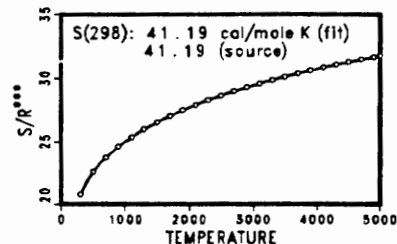
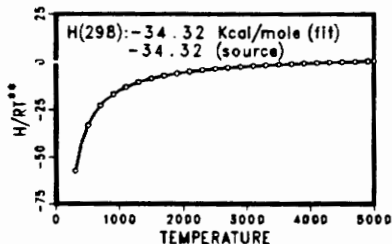
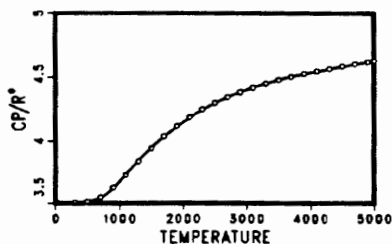
HYDROXYL, UNINEGATIVE ION

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|----------------|
| 0300-1000K   | 0.03390037E+02 | 0.07922381E-02 | -0.01943429E-04 | 0.02001769E-07 | -0.05702087E-11 | -0.01830493E+06 | 0.12498923E+01 |
| 1000-5000K   | 0.02846204E+02 | 0.10418347E-02 | -0.02416850E-05 | 0.02483215E-09 | -0.07775605E-14 | -0.01807280E+06 | 0.04422712E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: S

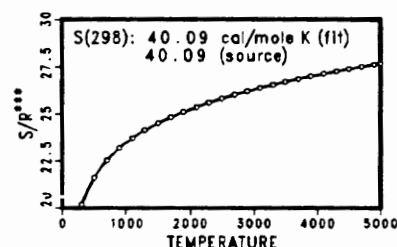
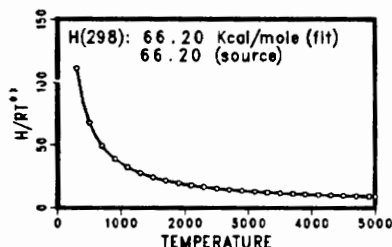
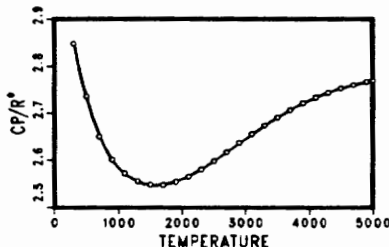
SULFUR, MONATOMIC

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.03187329E+02 | -0.15957763E-02 | 0.02005531E-04 | -0.15070814E-08 | 0.04931282E-11 | 0.03242259E+06 | 0.02414441E+02 |
| 1000-5000K   | 0.02902148E+02 | -0.05484546E-02 | 0.02764576E-05 | -0.05017114E-09 | 0.03150684E-13 | 0.03249423E+06 | 0.03838471E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: S(L)

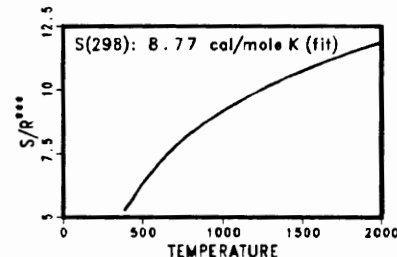
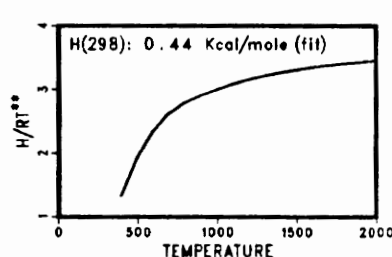
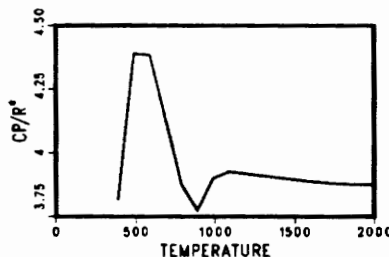
SULFUR

LIQUID

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0388-1000K   | -0.12706310E+02 | 0.09072521E+00 | -0.01695178E-02 | 0.13070636E-06 | -0.03527615E-09 | 0.12346069E+04  | 0.05621016E+03  |
| 1000-2000K   | 0.03603667E+02  | 0.09903341E-02 | -0.10114410E-05 | 0.04053632E-08 | -0.05667913E-12 | -0.08453839E+04 | -0.16344708E+02 |



Source: NASA FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: S(S)

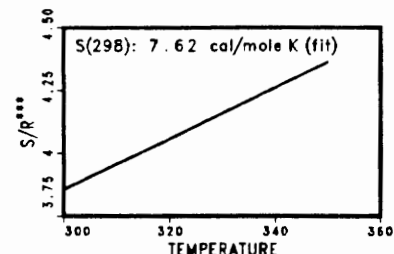
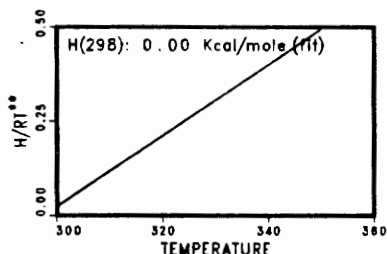
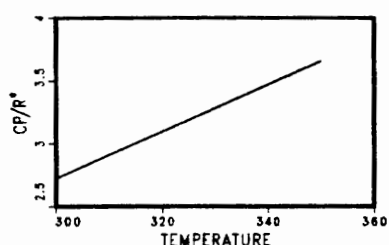
SULFUR

SOLID

As of: 12/01/86

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|-----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | -0.05063702E+02 | 0.02881935E-01 | -0.02133020E-03 | 0.08478786E-05 | -0.01734496E-07 | 0.07148263E+04 | 0.02871407E+03 |
| 1000-0388K   | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00  | 0.00000000E+00 | 0.00000000E+00 |



Source: NASA FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

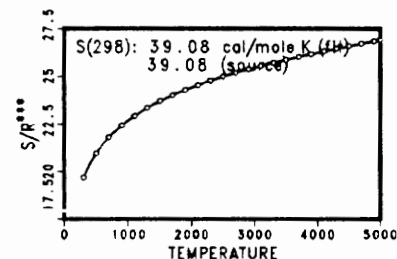
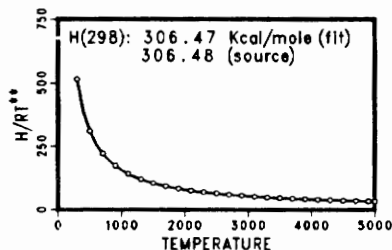
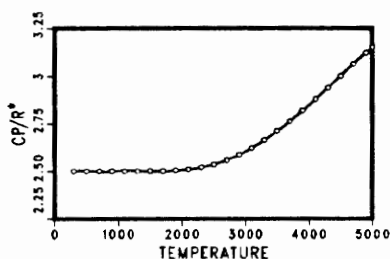
Species: S+

SULFUR, MONATOMIC, UNIPOSITIVE ION GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02366100E+02 | 0.09130767E-02 | -0.02140283E-04 | 0.02076177E-07 | -0.07133859E-11 | 0.15350910E+06 | 0.05993094E+02 |
| 1000-5000K   | 0.02404600E+02 | 0.02410908E-02 | -0.02041779E-05 | 0.06592945E-09 | -0.05756939E-13 | 0.15352225E+06 | 0.05924256E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

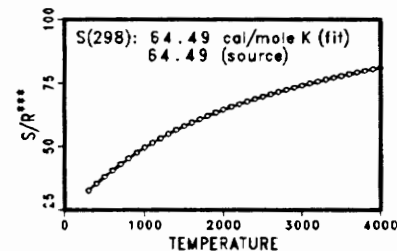
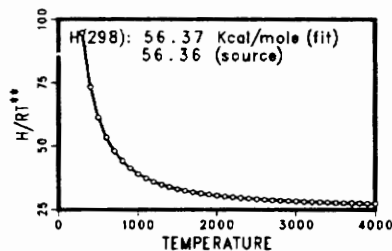
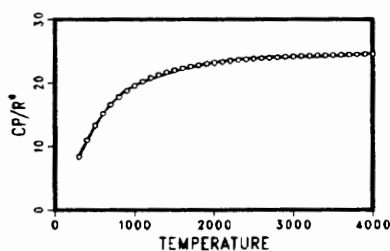
Species: S-TRIAZINE

GAS

As of: 4/16/87

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.04493492E+01 | 0.02728306E+00 | 0.02309304E-04  | -0.14968443E-07 | 0.04546753E-10 | 0.02703032E+06 | 0.02178518E+03  |
| 1000-4000K   | 0.13036170E+02 | 0.07711820E-01 | -0.07724374E-05 | -0.04385191E-08 | 0.08298992E-12 | 0.02251663E+06 | -0.04777676E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: S2

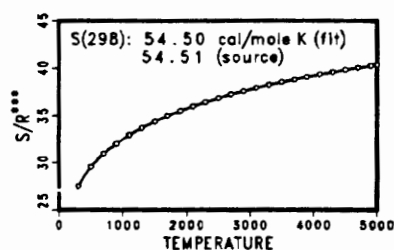
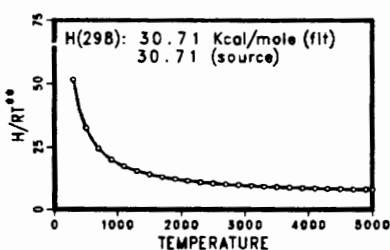
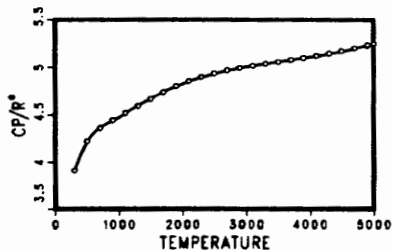
SULFUR, DIATOMIC

GAS

As of: 12/13/86

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6             | a7             |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.03157672E+02 | 0.03099480E-01 | -0.15607465E-05 | -0.13578905E-08 | 0.11374435E-11 | 0.14391873E+05 | 0.08596062E+02 |
| 1000-5000K   | 0.03904443E+02 | 0.06925733E-02 | -0.12330970E-06 | 0.08783809E-11  | 0.13746621E-14 | 0.14256933E+05 | 0.04956834E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SH

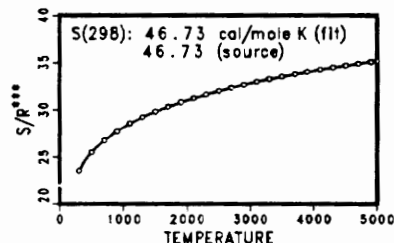
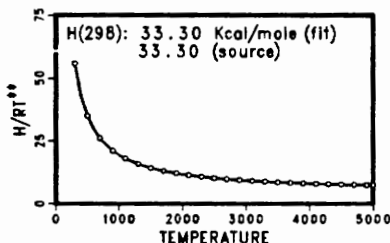
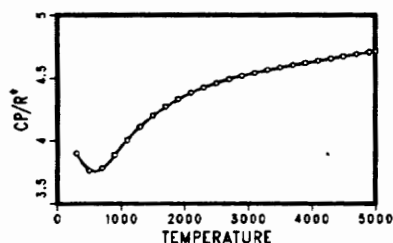
SULFUR MONOHYDRID

GAS

As of: 12/12/86

Fit

| Coefficients | a1             | a2              | a3              | a4             | a5              | a6             | a7             |
|--------------|----------------|-----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.04133326E+02 | -0.03787893E-02 | -0.02777854E-04 | 0.05370112E-07 | -0.02394006E-10 | 0.15558623E+05 | 0.16115348E+00 |
| 1000-5000K   | 0.03053810E+02 | 0.12588843E-02  | -0.04249169E-05 | 0.06929591E-09 | -0.04281691E-13 | 0.15882250E+05 | 0.05973551E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SI

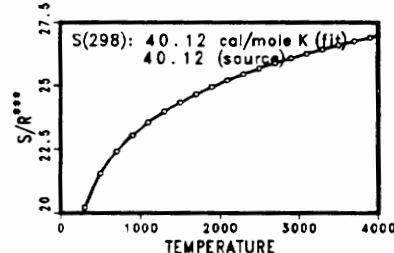
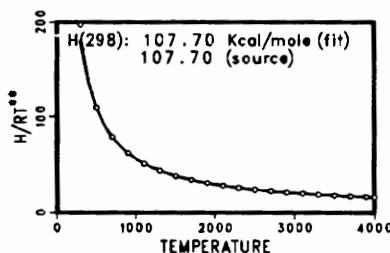
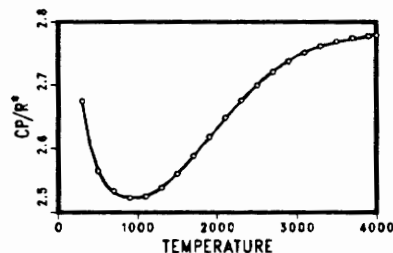
SILICON, MONATOMIC

GAS

As of: 3/29/89

Fit

| Coefficients | a1             | a2              | a3             | a4              | a5             | a6             | a7             |
|--------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.03113515E+02 | -0.02330991E-01 | 0.03518530E-04 | -0.02417573E-07 | 0.06391902E-11 | 0.05335061E+06 | 0.03009718E+02 |
| 1000-4000K   | 0.02775845E+02 | -0.06213257E-02 | 0.04843696E-05 | -0.12756146E-09 | 0.11344818E-13 | 0.05339790E+06 | 0.04543298E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: Si(L)

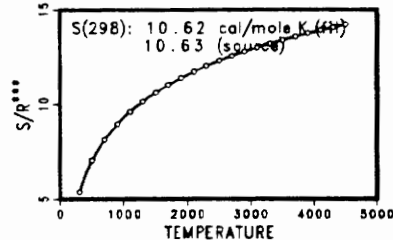
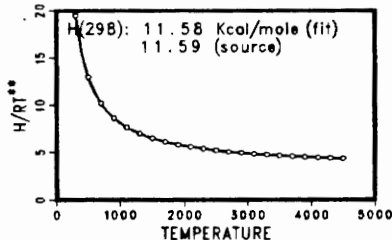
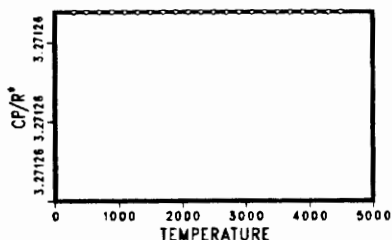
SILICON

LIQUID

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub> | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|----------------|----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03271263E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.04855058E+05 | -0.13290542E+02 |
| 1000-4500K   | 0.03271263E+02 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 | 0.04855057E+05 | -0.13290542E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: Si(NH<sub>2</sub>)<sub>3</sub>

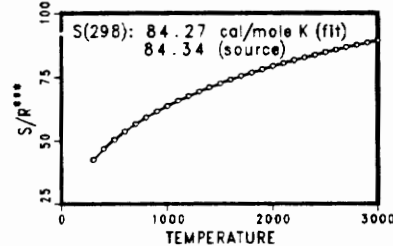
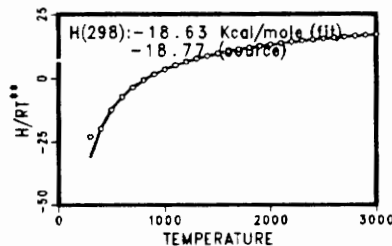
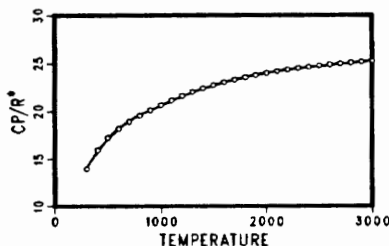
TRIAMINOSILYL

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.07598413E+02 | 0.02435266E+00 | -0.04296202E-04 | -0.01756006E-06 | 0.10501017E-10 | -0.12653434E+05 | -0.07808647E+02 |
| 1000-3000K   | 0.14065501E+02 | 0.07581744E-01 | -0.05168510E-05 | -0.06743626E-08 | 0.13979258E-12 | -0.14144028E+05 | -0.04063873E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: Si(NH<sub>2</sub>)<sub>4</sub>

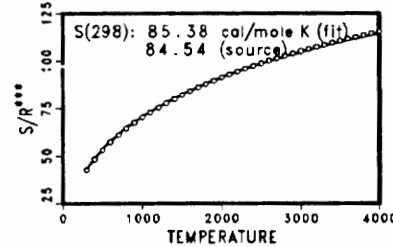
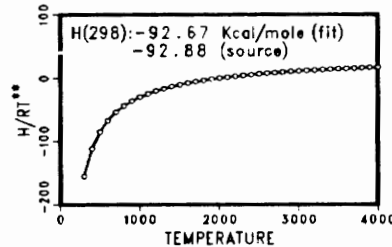
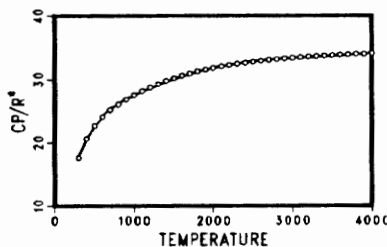
TETRAAMINOSILANE

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.08454529E+02 | 0.03465772E+00 | -0.04266782E-04 | -0.02495363E-06 | 0.13654663E-10 | -0.05061518E+06 | -0.15143013E+02 |
| 1000-4000K   | 0.02032107E+03 | 0.08289798E-01 | -0.07077612E-05 | -0.04340724E-08 | 0.07747068E-12 | -0.05389855E+06 | -0.07730464E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SI(S)

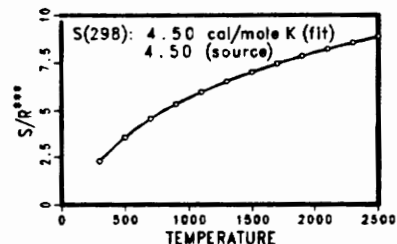
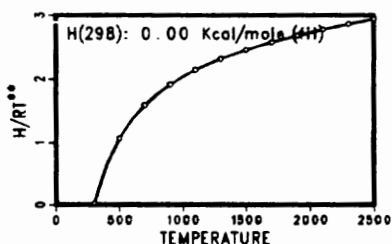
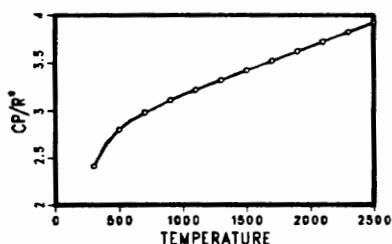
SILICON

SOLID

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.05746418E+01 | 0.10264855E-01 | -0.01775345E-03 | 0.14575000E-07 | -0.04491292E-10 | -0.04969951E+04 | -0.03400242E+02 |
| 1000-2500K   | 0.02530275E+02 | 0.08522433E-02 | -0.03223468E-05 | 0.12808208E-09 | -0.01850849E-12 | -0.08395197E+04 | -0.12514782E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SI2

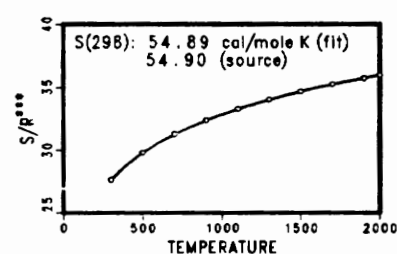
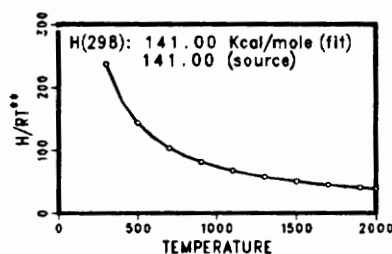
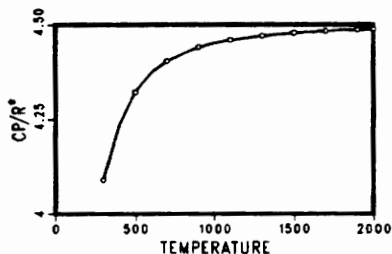
SILICON, DIATOMIC

GAS

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.02993750E+02 | 0.06053689E-01 | -0.10158575E-04 | 0.07909737E-07 | -0.02346083E-10 | 0.06987498E+06 | 0.09151741E+02 |
| 1000-2000K   | 0.04232196E+02 | 0.04315355E-02 | -0.02964833E-05 | 0.09823294E-09 | -0.12962688E-13 | 0.06964651E+06 | 0.03308527E+02 |



Source: SNLL FIT TO DATA GENERATE USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SI2C

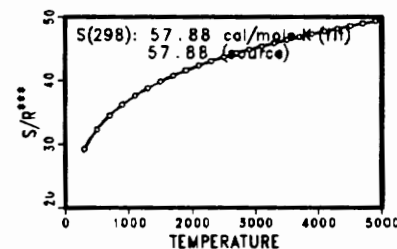
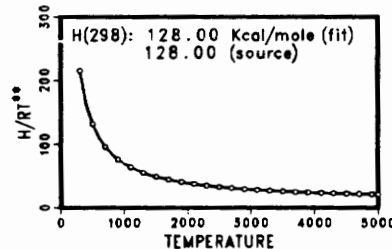
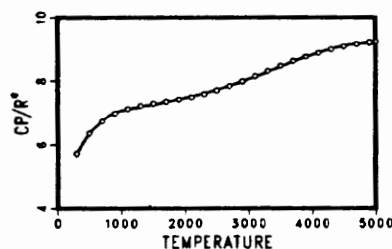
DISILICON CARBIDE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.04157246E+02 | 0.07031825E-01 | -0.07263033E-04 | 0.04633583E-07 | -0.14934475E-11 | 0.06292421E+06 | 0.03635125E+02  |
| 1000-5000K   | 0.06334110E+02 | 0.12102520E-02 | -0.06798289E-05 | 0.02244432E-08 | -0.02280177E-12 | 0.06227189E+06 | -0.07770097E+02 |



Source: SNLL FIT TO JANAF DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$



Species: SI2F6

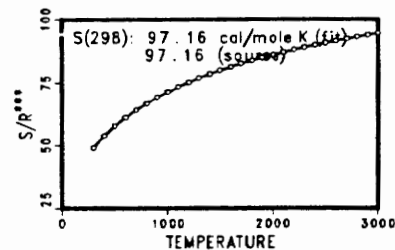
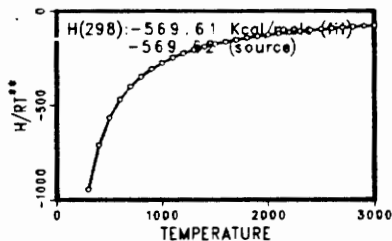
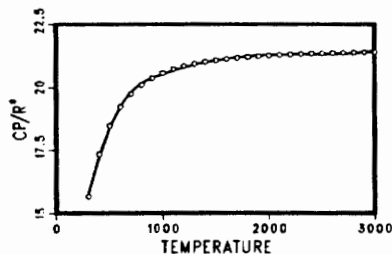
HEXAFLUORODISILANE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.09998134E+02 | 0.02170313E+00 | -0.03875091E-04 | -0.16702523E-07 | 0.09407529E-10 | -0.02905482E+07 | -0.14228863E+02 |
| 1000-3000K   | 0.01830047E+03 | 0.02868752E-01 | -0.04545576E-05 | -0.02497900E-08 | 0.06630658E-12 | -0.02928185E+07 | -0.05760425E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

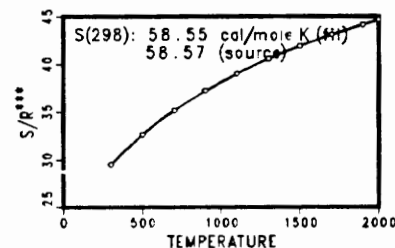
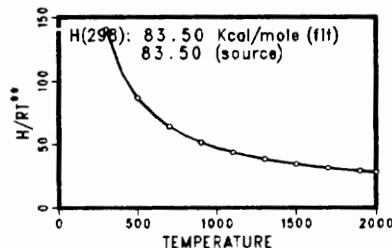
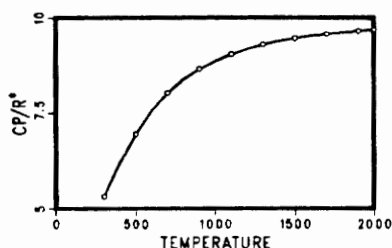
Species: SI2H2

GAS

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.16247229E+01 | 0.14871029E-01 | -0.08707160E-04 | -0.01699554E-09 | 0.10972211E-11 | 0.04095325E+06 | 0.16165730E+02  |
| 1000-2000K   | 0.05778180E+02 | 0.04070596E-01 | -0.04259125E-05 | -0.07920228E-08 | 0.02379752E-11 | 0.03980520E+06 | -0.05392375E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

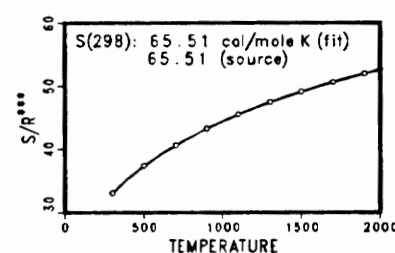
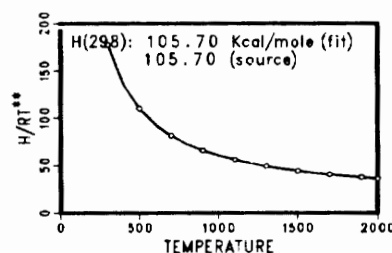
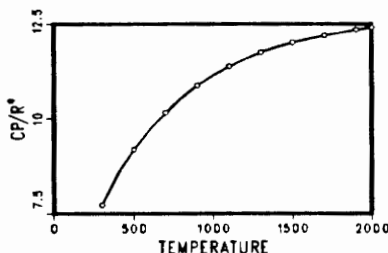
Species: SI2H3

GAS

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03335404E+02 | 0.02155614E+00 | -0.02933937E-03 | 0.02287784E-06  | -0.07272827E-10 | 0.05146157E+06 | 0.08656853E+02  |
| 1000-2000K   | 0.07257627E+02 | 0.05123859E-01 | -0.07633465E-05 | -0.06662471E-08 | 0.02053052E-11  | 0.05062055E+06 | -0.10314127E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

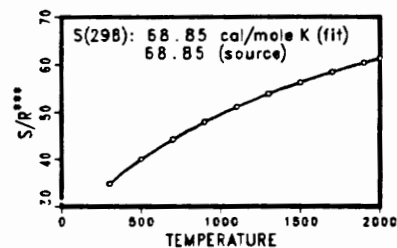
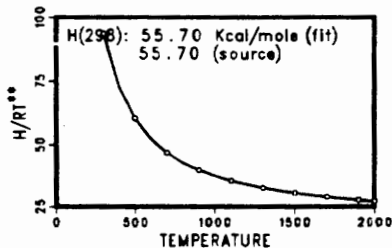
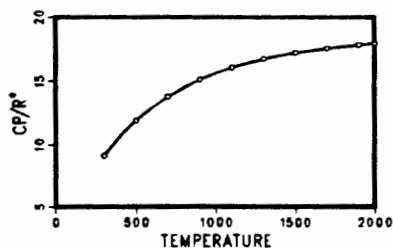
Species: Si2H5

GAS

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.15788481E+01 | 0.03549382E+00 | -0.04267511E-03 | 0.03059177E-06  | -0.09360425E-10 | 0.02630549E+06 | 0.16720734E+02  |
| 1000-2000K   | 0.08451010E+02 | 0.09286371E-01 | -0.10911831E-05 | -0.14423673E-08 | 0.04250824E-11  | 0.02472718E+06 | -0.01710331E+03 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

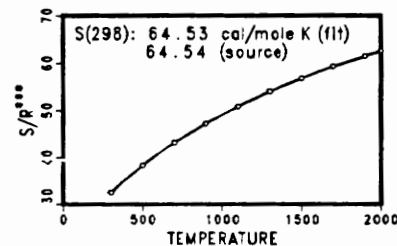
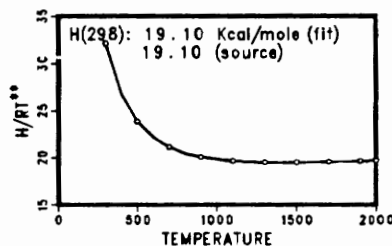
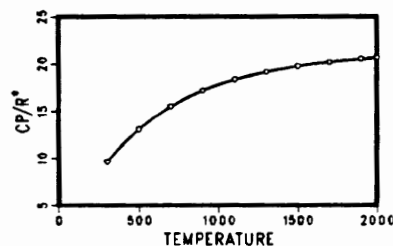
Species: Si2H6

GAS

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.05301921E+01 | 0.04184055E+00 | -0.04685249E-03 | 0.03179525E-06  | -0.09484526E-10 | 0.07950597E+05 | 0.01880453E+03  |
| 1000-2000K   | 0.08882090E+02 | 0.11513955E-01 | -0.12162159E-05 | -0.01905085E-07 | 0.05542379E-11  | 0.05967241E+05 | -0.02265611E+03 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: Si3

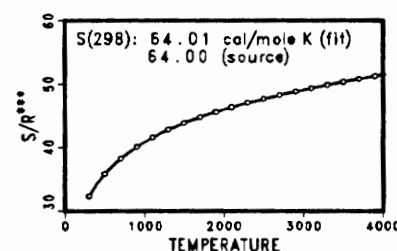
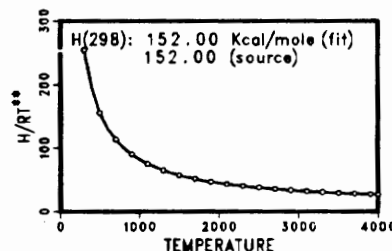
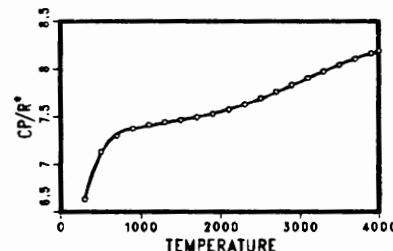
SILICON, TRIATOMIC

GAS

As of: 3/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.05312161E+02 | 0.05920180E-01 | -0.05075224E-04 | 0.05303866E-08 | 0.07031630E-11  | 0.07469501E+06 | 0.04036452E+01  |
| 1000-4000K   | 0.07021584E+02 | 0.06981538E-02 | -0.04818729E-05 | 0.01720754E-08 | -0.01927024E-12 | 0.07429956E+06 | -0.08179232E+02 |



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

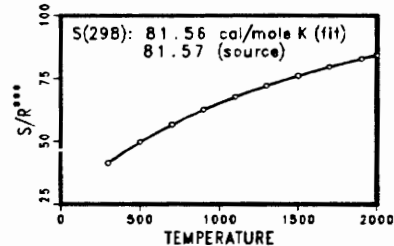
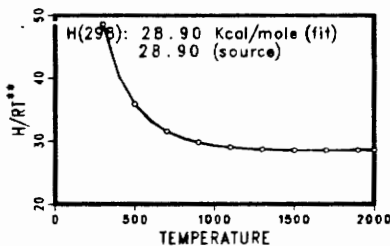
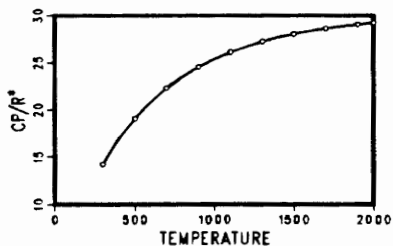
Species: SI3H8

GAS

As of: 9/05/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.06319791E+01 | 0.06412995E+00 | -0.07772444E-03 | 0.05486969E-06  | -0.16460971E-10 | 0.12092580E+05 | 0.02133318E+03  |
| 1000-2000K   | 0.13422770E+02 | 0.15636323E-01 | -0.01936565E-04 | -0.02388329E-07 | 0.07120030E-11  | 0.09165887E+05 | -0.04163000E+03 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SI3N4(A)

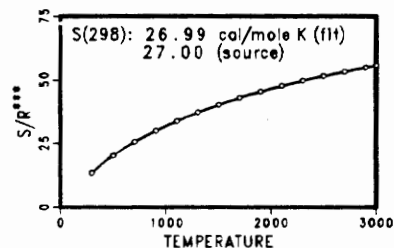
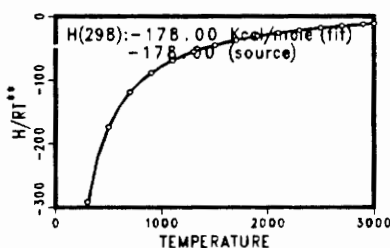
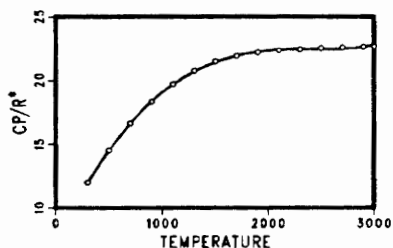
SILICON NITRIDE, ALPHA

SOLID

As of: 4/25/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.06631384E+02 | 0.02293928E+00 | -0.02152875E-03 | 0.01766237E-06  | -0.06632214E-10 | -0.09241684E+06 | -0.03021795E+03 |
| 1000-3000K   | 0.09667453E+02 | 0.11927212E-01 | -0.01709281E-04 | -0.10846074E-08 | 0.02713018E-11  | -0.09324734E+06 | -0.04556492E+03 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIC

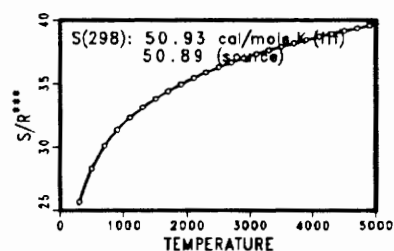
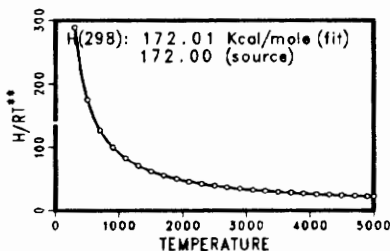
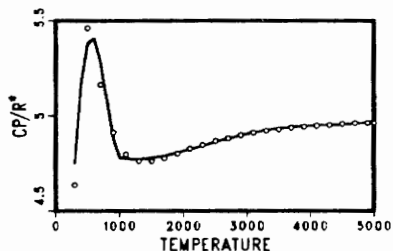
SILICON CARBIDE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|-----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02427812E+02 | 0.09551934E-01  | -0.02796633E-04 | -0.13600122E-07 | 0.09196322E-10 | 0.08546512E+06 | 0.09179253E+02  |
| 1000-5000K   | 0.05024270E+02 | -0.04920894E-02 | 0.03109315E-05  | -0.06901344E-09 | 0.05215735E-13 | 0.08531026E+06 | -0.02476798E+02 |



Source: SNLL FIT TO JANAF DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIC(B)

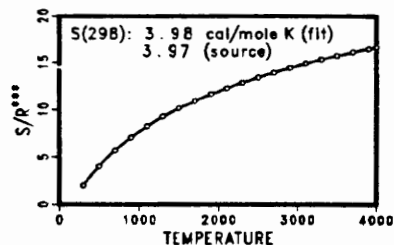
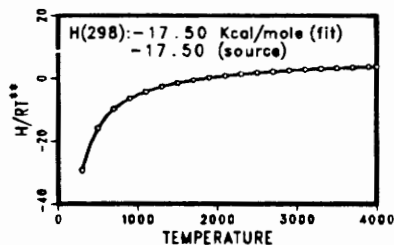
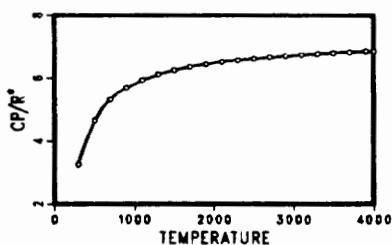
SILICON CARBIDE, BETA

SOLID

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub>  | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|-----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | -0.03551395E+01 | 0.15998806E-01 | -0.13933268E-04 | 0.03314914E-07 | 0.07825957E-11  | -0.09294352E+05 | -0.15153885E+00 |
| 1000-4000K   | 0.03548056E+02  | 0.03636817E-01 | -0.01734872E-04 | 0.03912869E-08 | -0.03337952E-12 | -0.10188585E+05 | -0.01967253E+03 |



Source: SNLL FIT TO JANNAF DATA

$$\begin{aligned}
 * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\
 ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7
 \end{aligned}$$

Species: SIC2

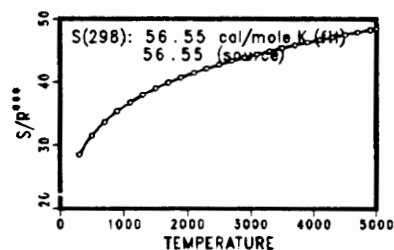
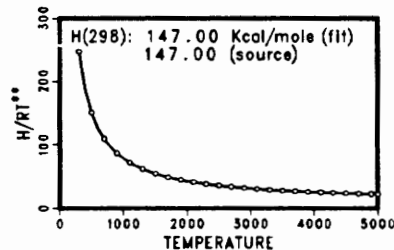
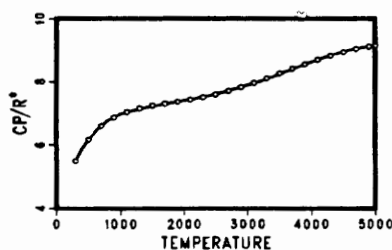
SILICON DICARBIDE

GAS

As of: 11/29/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.03647724E+02 | 0.08765100E-01 | -0.10796686E-04 | 0.07974287E-07 | -0.02617042E-10 | 0.07258578E+06 | 0.05481049E+02  |
| 1000-5000K   | 0.05753725E+02 | 0.02067546E-01 | -0.11325346E-05 | 0.03106456E-08 | -0.02799936E-12 | 0.07200461E+06 | -0.05294926E+02 |



Source: SNLL FIT TO JANNAF DATA

$$\begin{aligned}
 * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\
 ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7
 \end{aligned}$$

Species: SICL

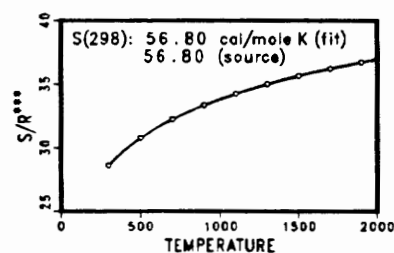
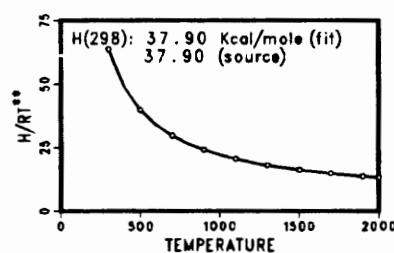
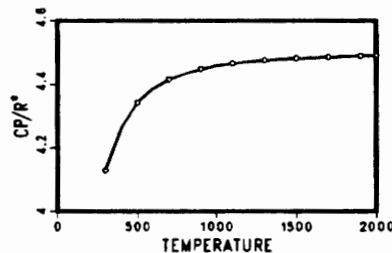
SILICON MONOCHLORIDE

GAS

As of: 12/19/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03096406E+02 | 0.05738623E-01 | -0.09740903E-04 | 0.07643597E-07 | -0.02279178E-10 | 0.01796794E+06 | 0.09603212E+02 |
| 1000-2000K   | 0.04258459E+02 | 0.04020317E-02 | -0.02888145E-05 | 0.10097771E-09 | -0.14110117E-13 | 0.01775613E+06 | 0.04134521E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned}
 * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\
 ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7
 \end{aligned}$$

Species: SICL2

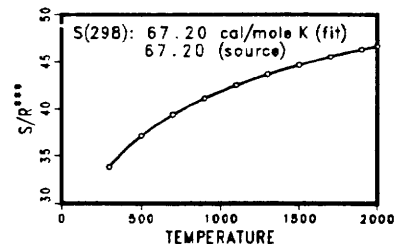
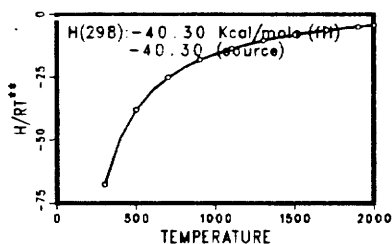
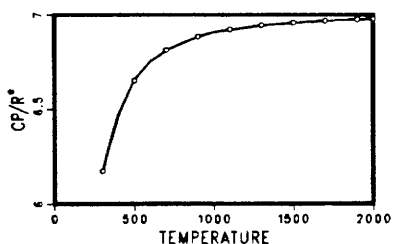
DICHLOROSILYLENE

GAS

As of: 12/19/86

Fit

| Coefficients | a1             | a2             | a3              | a4             | a5              | a6              | a7              |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.0382666E+02  | 0.13082964E-01 | -0.02234087E-03 | 0.01760741E-06 | -0.05267404E-10 | -0.02183869E+06 | 0.08965448E+02  |
| 1000-2000K   | 0.06491204E+02 | 0.08242384E-02 | -0.05767737E-05 | 0.01972405E-08 | -0.02713757E-12 | -0.02232408E+06 | -0.03570531E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: SICL2H2

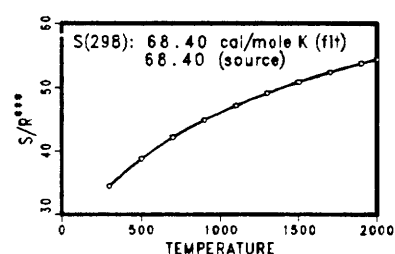
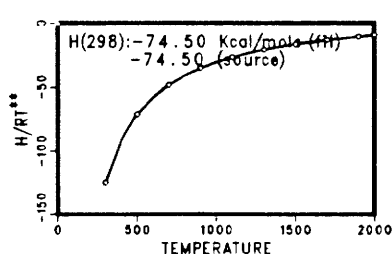
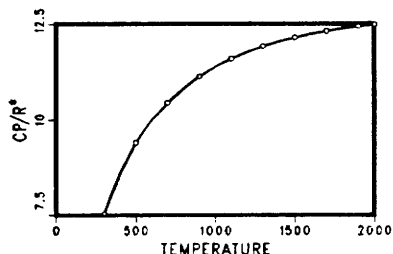
DICHLOROSILANE

GAS

As of: 12/19/86

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5              | a6              | a7              |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.11002086E+01 | 0.03262361E+00 | -0.04691994E-03 | 0.03494565E-06  | -0.10362847E-10 | -0.03892086E+06 | 0.02022693E+03  |
| 1000-2000K   | 0.07727079E+02 | 0.05034188E-01 | -0.10957459E-05 | -0.04419587E-08 | 0.16311241E-12  | -0.04028605E+06 | -0.11708156E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: SICL3

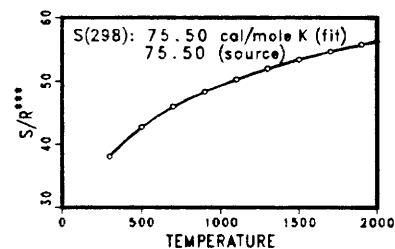
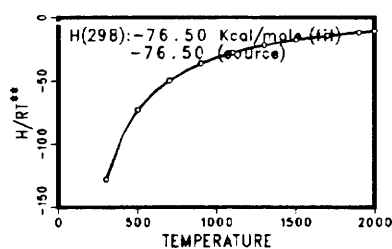
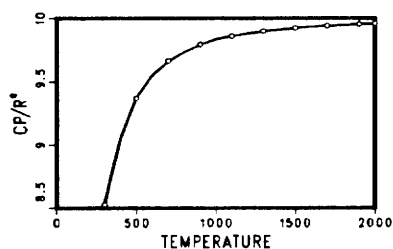
TRICHLOROSILYL RADICAL

GAS

As of: 12/19/86

Fit

| Coefficients | a1             | a2             | a3              | a4             | a5              | a6              | a7              |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.04485690E+02 | 0.02241754E+00 | -0.03794196E-03 | 0.02973183E-06 | -0.08861335E-10 | -0.04055264E+06 | 0.07198771E+02  |
| 1000-2000K   | 0.09098097E+02 | 0.14053526E-02 | -0.09317005E-05 | 0.02982296E-08 | -0.03822010E-12 | -0.04140193E+06 | -0.14550117E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: SICL3H

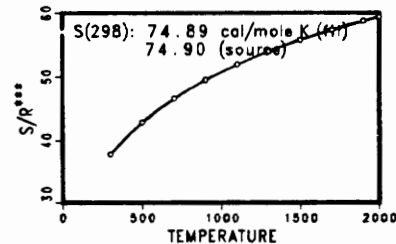
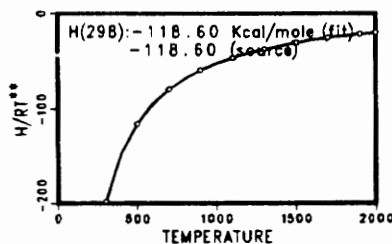
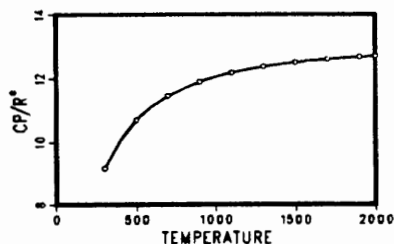
TRICHLOROSILANE

GAS

As of: 12/19/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02883769E+02 | 0.03308240E+00 | -0.05169241E-03 | 0.03949918E-06  | -0.11721043E-10 | -0.06163323E+06 | 0.13374664E+02  |
| 1000-2000K   | 0.09663121E+02 | 0.03563367E-01 | -0.12149114E-05 | -0.16090094E-10 | 0.05641710E-12  | -0.06295557E+06 | -0.01894777E+03 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SICL4

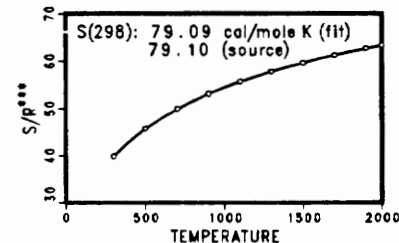
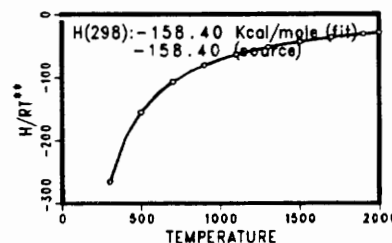
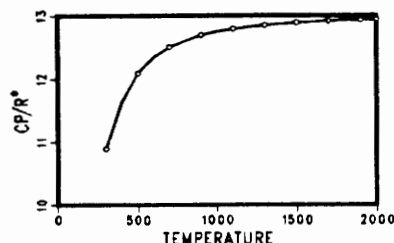
TETRACHLOROSILANE

GAS

As of: 12/19/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.05252110E+02 | 0.03122067E+00 | -0.05254593E-03 | 0.04102707E-06 | -0.12199071E-10 | -0.08228177E+06 | 0.02575727E+02  |
| 1000-2000K   | 0.11709377E+02 | 0.01972091E-01 | -0.12690771E-05 | 0.03900188E-08 | -0.04756468E-12 | -0.08347808E+06 | -0.02791153E+03 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SICLH3

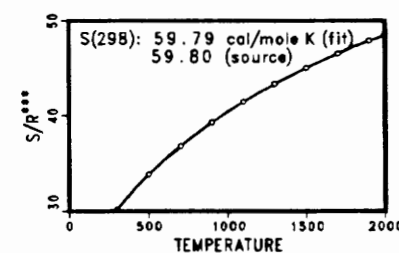
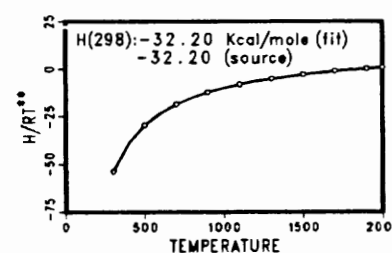
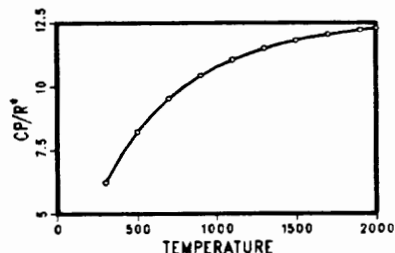
CHLOROSILANE

GAS

As of: 12/19/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.05057173E+01 | 0.02703377E+00 | -0.03301474E-03 | 0.02302732E-06  | -0.06778703E-10 | -0.01730819E+06 | 0.02043167E+03  |
| 1000-2000K   | 0.05964237E+02 | 0.06278087E-01 | -0.08205634E-05 | -0.09280558E-08 | 0.02796642E-11  | -0.01854309E+06 | -0.06395305E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIF

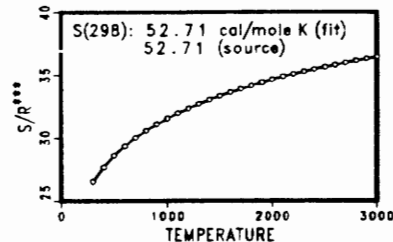
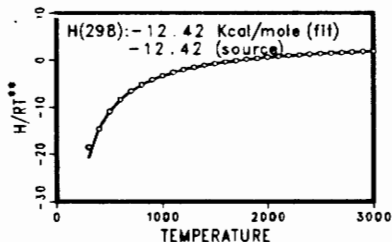
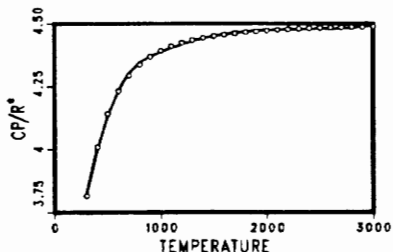
FLUROSILYLIDYNE

GAS

As of: 4/24/89

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6              | a7             |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|----------------|
| 0300-1000K   | 0.03144947E+02 | 0.02588557E-01 | -0.05795912E-05 | -0.01807278E-07 | 0.10411718E-11 | -0.07294439E+05 | 0.07876774E+02 |
| 1000-3000K   | 0.04120066E+02 | 0.03548820E-02 | -0.07200222E-06 | -0.02190434E-09 | 0.06764591E-13 | -0.07561378E+05 | 0.02784246E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: SIF(NH2)2

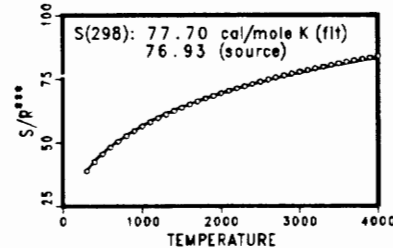
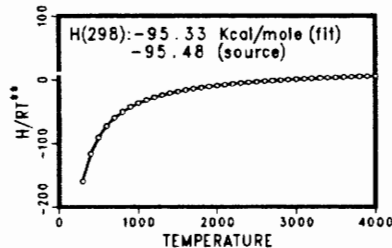
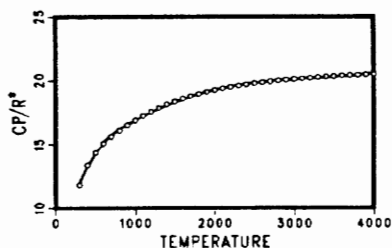
DIAMINOFLUROSILYL RADICAL

GAS

As of: 2/27/90

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6              | a7              |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.07210094E+02 | 0.01764697E+00 | -0.02542059E-04 | -0.12422138E-07 | 0.06989787E-10 | -0.05086706E+06 | -0.07024622E+02 |
| 1000-4000K   | 0.12879436E+02 | 0.04598535E-01 | -0.04004440E-05 | -0.02374189E-08 | 0.04255211E-12 | -0.05238278E+06 | -0.03653418E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: SIF(NH2)3

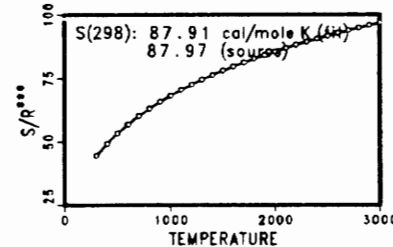
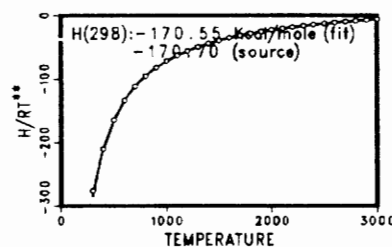
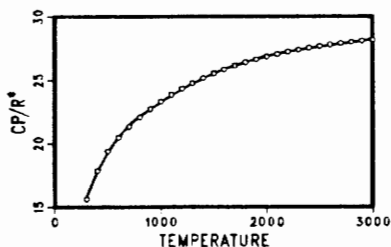
TRIAMINOFLUROSILANE

GAS

As of: 4/24/89

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6              | a7              |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.08388268E+02 | 0.02746622E+00 | -0.04455674E-04 | -0.01955732E-06 | 0.11407210E-10 | -0.08947806E+06 | -0.11381777E+02 |
| 1000-3000K   | 0.16111795E+02 | 0.08329222E-01 | -0.06023787E-05 | -0.07470125E-08 | 0.15707311E-12 | -0.09137007E+06 | -0.05098123E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * CP/R &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \\ ** H/RT &= a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7 \end{aligned}$$

Species: SIF2

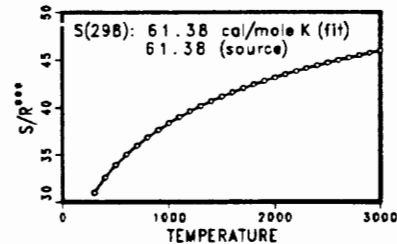
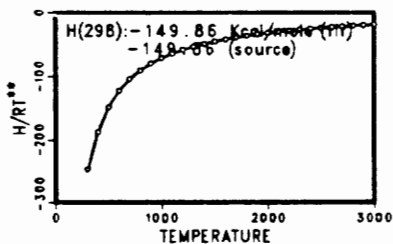
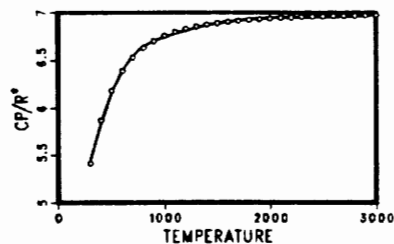
DIFLUOROSILYLENE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.03845345E+02 | 0.06038465E-01 | -0.11677323E-05 | -0.04579553E-07 | 0.02607414E-10 | -0.07681633E+06 | 0.07272983E+02  |
| 1000-3000K   | 0.06142470E+02 | 0.07807974E-02 | -0.13393119E-06 | -0.06264839E-09 | 0.01725138E-12 | -0.07744042E+06 | -0.04712327E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: SIF2(NH2)2

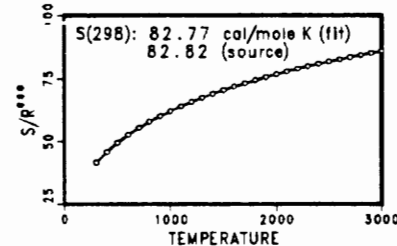
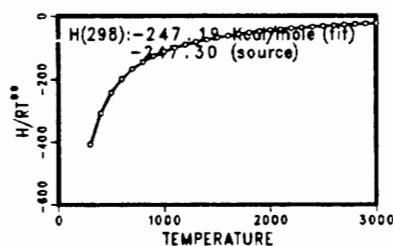
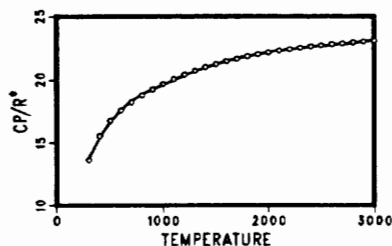
DIFLUORODIAMINOSILANE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.07634268E+02 | 0.02315843E+00 | -0.04193827E-04 | -0.01715350E-06 | 0.10164619E-10 | -0.12764102E+06 | -0.08419031E+02 |
| 1000-3000K   | 0.14414775E+02 | 0.06110646E-01 | -0.04871145E-05 | -0.05455935E-08 | 0.11727140E-12 | -0.12927572E+06 | -0.04308682E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

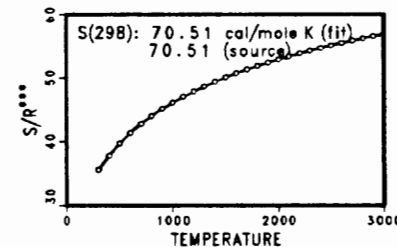
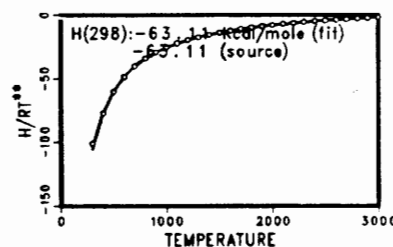
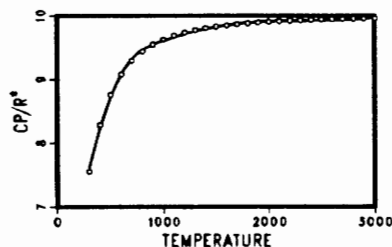
Species: SIF2N

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.05102583E+02 | 0.09456606E-01 | -0.01819383E-04 | -0.07309616E-07 | 0.04178902E-10 | -0.03367293E+06 | 0.03734423E+02  |
| 1000-3000K   | 0.08687337E+02 | 0.11934885E-02 | -0.01992660E-05 | -0.09951333E-09 | 0.02704383E-12 | -0.03463832E+06 | -0.14940526E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$



Species: SIF2NH2

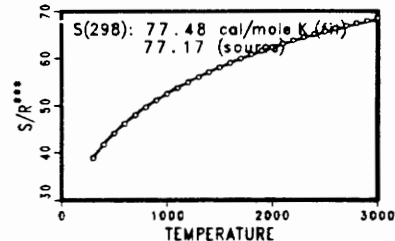
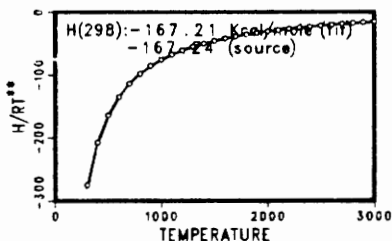
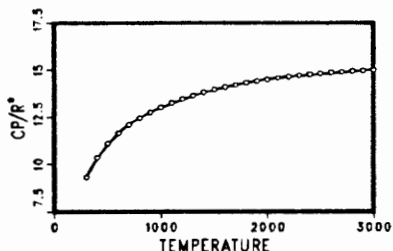
DIFLUOROAMINOSILYL

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.05890444E+02 | 0.12851282E-01 | -0.01863556E-04 | -0.08718963E-07 | 0.04848951E-10 | -0.08644527E+06 | 0.01756162E+02  |
| 1000-3000K   | 0.09872415E+02 | 0.03722112E-01 | -0.03271338E-05 | -0.03321674E-08 | 0.07293692E-12 | -0.08751628E+06 | -0.01899095E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIF3

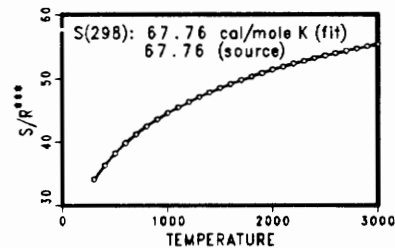
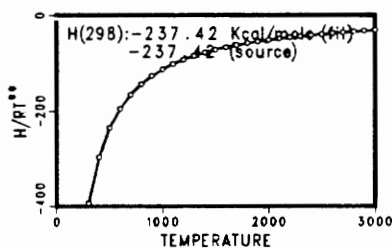
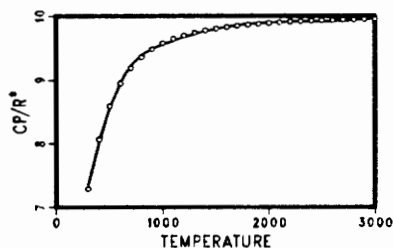
TRIFLUOROSILYL

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.04662868E+02 | 0.10087878E-01 | -0.01805544E-04 | -0.07769299E-07 | 0.04377851E-10 | -0.12129652E+06 | 0.04672966E+02  |
| 1000-3000K   | 0.08524790E+02 | 0.13237924E-02 | -0.02104278E-05 | -0.11495040E-09 | 0.03055301E-12 | -0.12235223E+06 | -0.15502343E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIF3NH

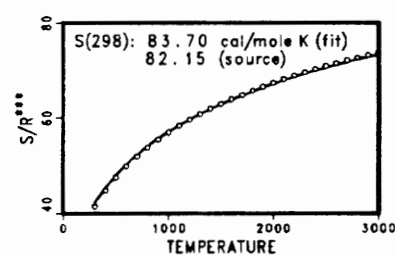
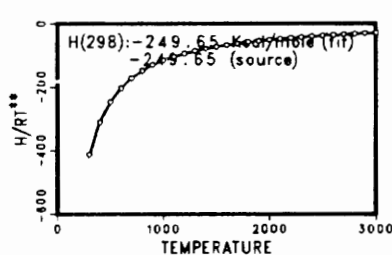
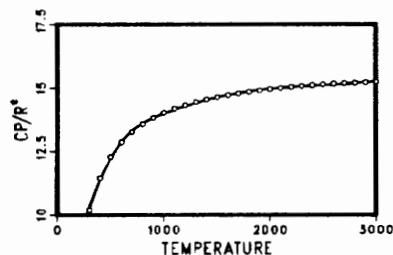
TRIFLUOROSILYLAMIDOGEN

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.06013822E+02 | 0.15977294E-01 | -0.02791466E-04 | -0.12141200E-07 | 0.06927415E-10 | -0.12809741E+06 | 0.03316770E+02  |
| 1000-3000K   | 0.11637665E+02 | 0.02880768E-01 | -0.03357310E-05 | -0.02584594E-08 | 0.06162371E-12 | -0.12958909E+06 | -0.02590717E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIF3NH2

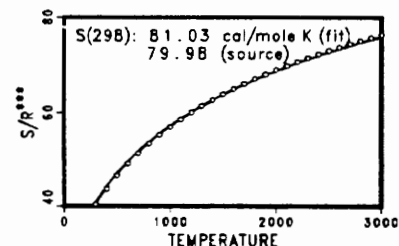
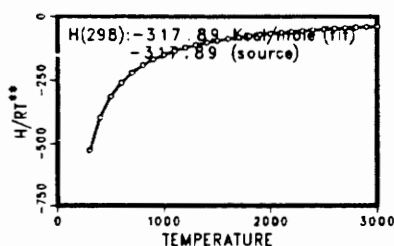
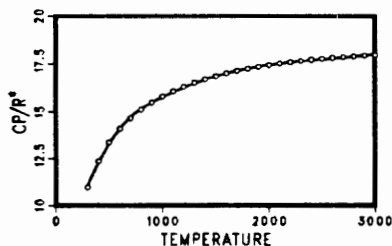
TRIFLUOROSILYLAMINE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.06229403E+02 | 0.01778015E+00 | -0.02612304E-04 | -0.12672434E-07 | 0.07044556E-10 | -0.16258489E+06 | 0.02045440E+01  |
| 1000-3000K   | 0.12109636E+02 | 0.04383282E-01 | -0.04142245E-05 | -0.03989090E-08 | 0.08958954E-12 | -0.16417679E+06 | -0.03046928E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIF3NHSIH3

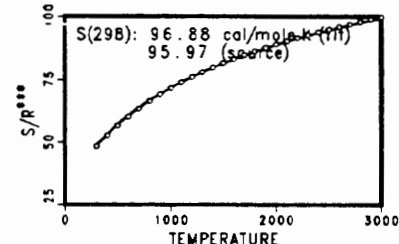
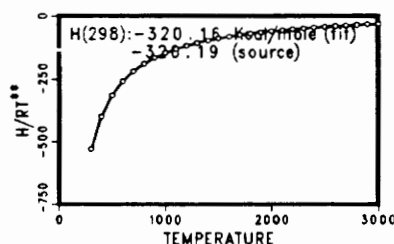
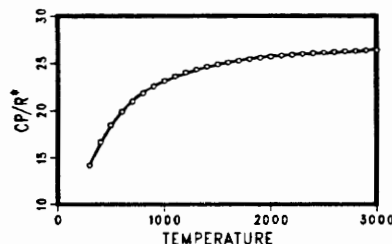
TRIFLUOROSILYL-SILYLAMINE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.06216046E+02 | 0.02939330E+00 | -0.02717745E-04 | -0.01982877E-06 | 0.10027676E-10 | -0.16422818E+06 | 0.04858261E+02  |
| 1000-3000K   | 0.16699406E+02 | 0.07789784E-01 | -0.08110570E-05 | -0.07650199E-08 | 0.01773956E-11 | -0.16734123E+06 | -0.05080007E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

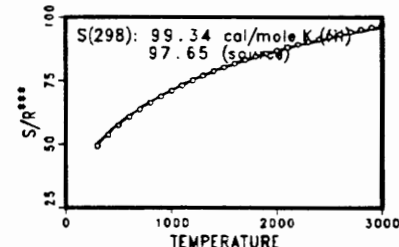
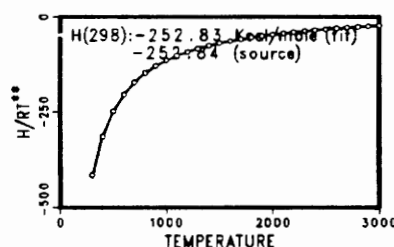
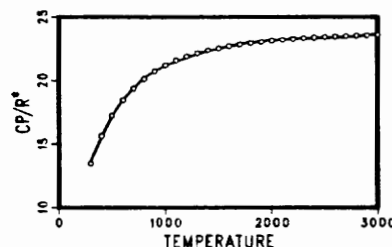
Species: SIF3NSIH3

TRIFLUOROSILYL-SILYLAMIDOGEN GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.06404371E+02 | 0.02601982E+00 | -0.02491543E-04 | -0.01769542E-06 | 0.08919883E-10 | -0.13025197E+06 | 0.06002945E+02  |
| 1000-3000K   | 0.15991462E+02 | 0.06371085E-01 | -0.07256823E-05 | -0.06292690E-08 | 0.14951566E-12 | -0.13311576E+06 | -0.04495265E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIF4

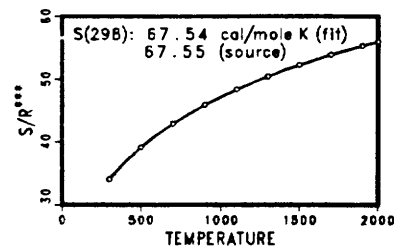
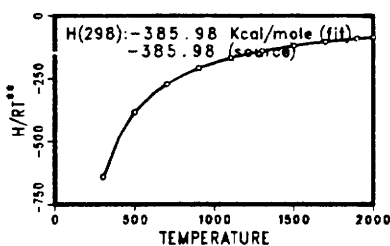
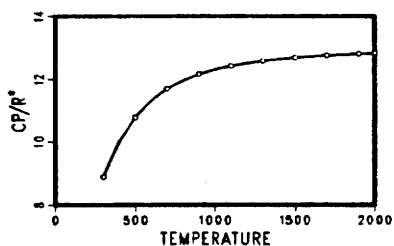
SILICON TETRAFLUORIDE

GAS

As of: 4/13/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02147416E+02 | 0.03402219E+00 | -0.04756873E-03 | 0.03252196E-06  | -0.08819304E-10 | -0.01960449E+07 | 0.13463150E+02  |
| 1000-2000K   | 0.09985301E+02 | 0.03532637E-01 | -0.11973776E-05 | -0.10365486E-09 | 0.08661585E-12  | -0.01977199E+07 | -0.02472643E+03 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIFH3

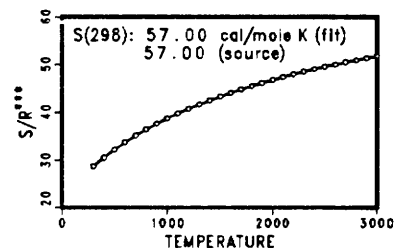
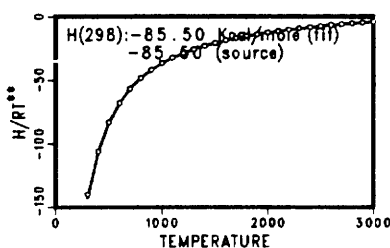
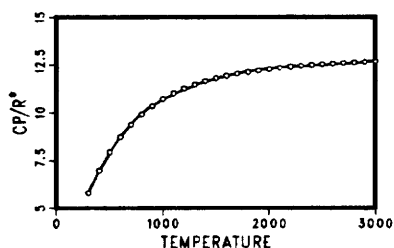
FLUOROSILANE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.02032189E+02 | 0.13413632E-01 | -0.02806381E-05 | -0.07803291E-07 | 0.03337474E-10 | -0.04421627E+06 | 0.13187677E+02  |
| 1000-3000K   | 0.06799678E+02 | 0.04747086E-01 | -0.04767066E-05 | -0.04814665E-08 | 0.11077613E-12 | -0.04577024E+06 | -0.12614326E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

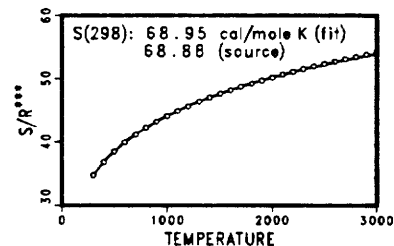
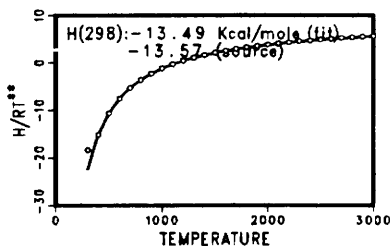
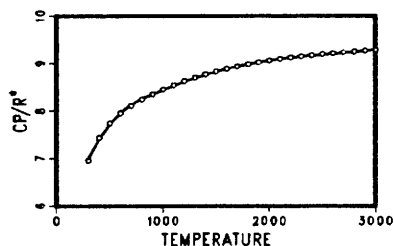
Species: SIFNH

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.05390691E+02 | 0.06071319E-01 | -0.13594903E-05 | -0.04267435E-07 | 0.02603153E-10 | -0.08644237E+05 | 0.02272064E+02  |
| 1000-3000K   | 0.07163298E+02 | 0.15213245E-02 | -0.15363371E-06 | -0.11959331E-09 | 0.02684099E-12 | -0.09065496E+05 | -0.06764144E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIFNH2

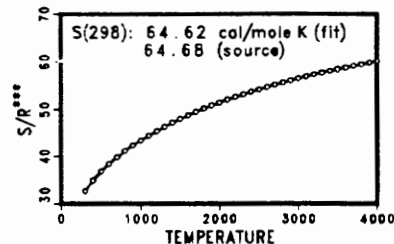
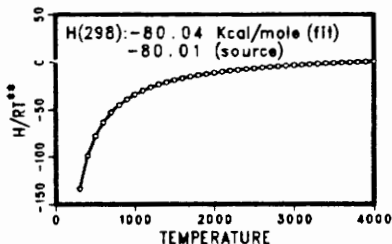
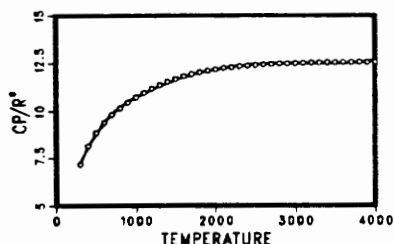
AMINOFLUOROSILYLENE

GAS

As of: 2/27/90

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.04214050E+02 | 0.11054231E-01 | -0.10147254E-05 | -0.07143728E-07 | 0.03634922E-10 | -0.04200629E+06 | 0.05318889E+02  |
| 1000-4000K   | 0.08017582E+02 | 0.03209103E-01 | -0.03361364E-05 | -0.01796536E-08 | 0.03385552E-12 | -0.04313426E+06 | -0.14870236E+02 |



Source: SNL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: SIH

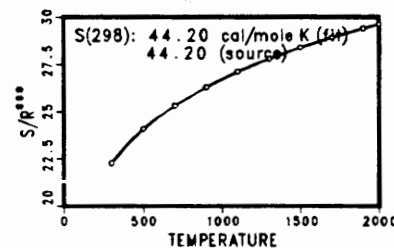
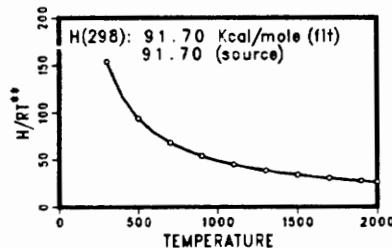
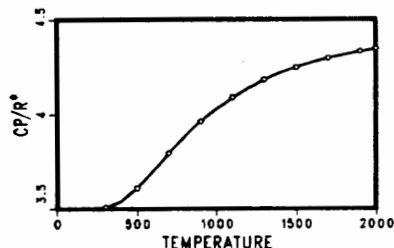
SILICON MONOHYDRIDE

GAS

As of: 12/19/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub>  | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|-----------------|----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.03836009E+02 | -0.02702656E-01 | 0.06849070E-04 | -0.05424184E-07 | 0.14721313E-11 | 0.04507593E+06 | 0.09350778E+01 |
| 1000-2000K   | 0.03110430E+02 | 0.10949460E-02  | 0.02898628E-06 | -0.02745104E-08 | 0.07051799E-12 | 0.04516897E+06 | 0.04193487E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: SIH2

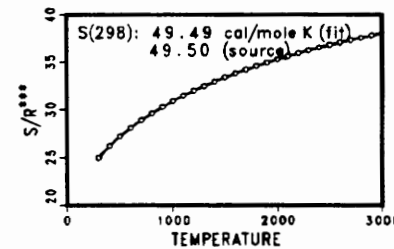
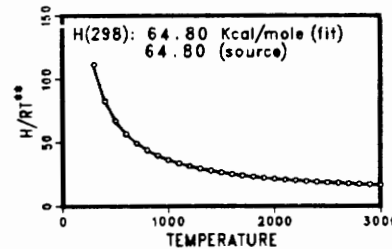
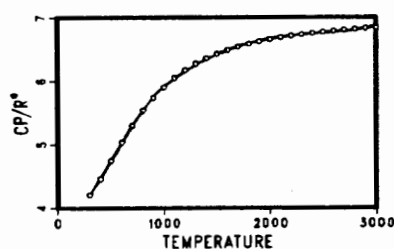
SILYLENE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03475092E+02 | 0.02139338E-01 | 0.07672305E-05  | 0.05217668E-08  | -0.09898824E-11 | 0.03147397E+06 | 0.04436585E+02 |
| 1000-3000K   | 0.04142390E+02 | 0.02150191E-01 | -0.02190730E-05 | -0.02073725E-08 | 0.04741018E-12  | 0.03110483E+06 | 0.02930745E+01 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned}
 * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\
 ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\
 *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7
 \end{aligned}$$

Species: SIH2CL

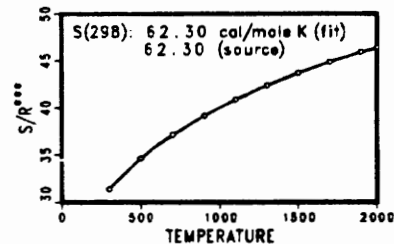
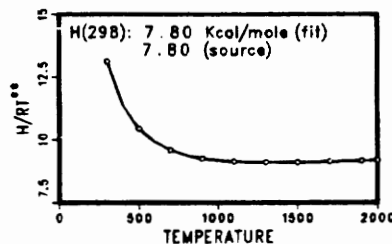
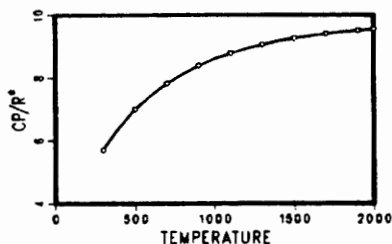
CHLOROSILYL RADICAL

GAS

As of: 12/19/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.01699256E+02 | 0.01961407E+00 | -0.02622973E-03 | 0.01936416E-06  | -0.05846399E-10 | 0.02743661E+05 | 0.01683132E+03  |
| 1000-2000K   | 0.05555901E+02 | 0.04046479E-01 | -0.06561751E-05 | -0.05027548E-08 | 0.15991101E-12  | 0.01912428E+05 | -0.01906889E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIH2F

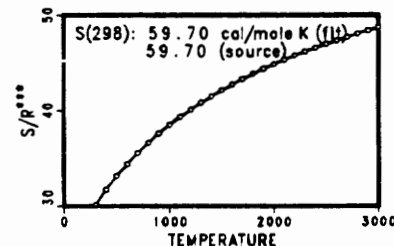
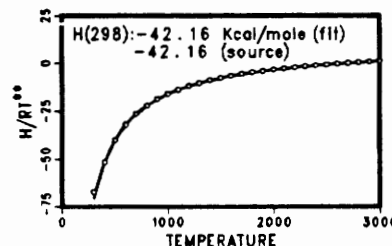
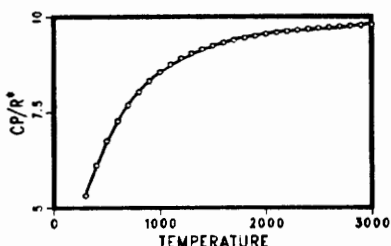
FLUOROSILYL

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.02782566E+02 | 0.09148257E-01 | -0.04186787E-05 | -0.05388971E-07 | 0.02412133E-10 | -0.02244201E+06 | 0.11528536E+02  |
| 1000-3000K   | 0.06020398E+02 | 0.03074039E-01 | -0.03248886E-05 | -0.03052243E-08 | 0.07098090E-12 | -0.02347670E+06 | -0.05919595E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIH2F2

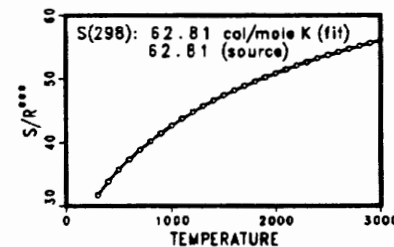
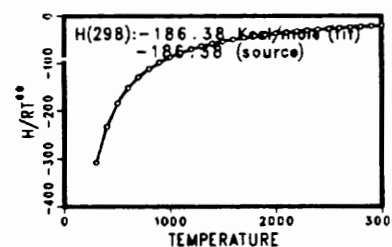
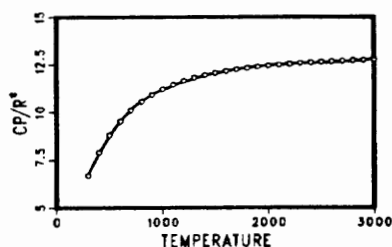
DIFLUOROSILANE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.02701455E+02 | 0.14565451E-01 | -0.11633003E-05 | -0.09685830E-07 | 0.04769590E-10 | -0.09522440E+06 | 0.12006887E+02  |
| 1000-3000K   | 0.07997762E+02 | 0.03911538E-01 | -0.04222679E-05 | -0.03913812E-08 | 0.09171569E-12 | -0.09682880E+06 | -0.16223999E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIH3

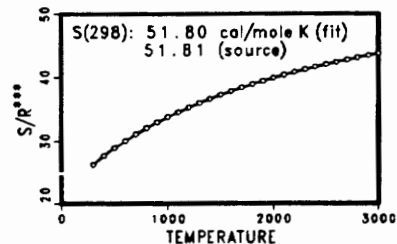
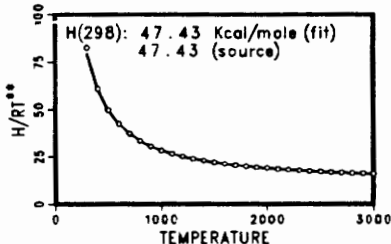
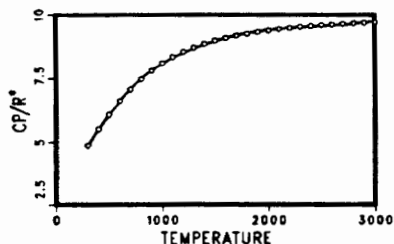
SILYL RADICAL

GAS

As of: 4/24/89

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6             | a7              |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02946733E+02 | 0.06466763E-01 | 0.05991653E-05  | -0.02218413E-07 | 0.03052669E-11 | 0.02270173E+06 | 0.07347948E+02  |
| 1000-3000K   | 0.05015906E+02 | 0.03732750E-01 | -0.03609053E-05 | -0.03729193E-08 | 0.08468491E-12 | 0.02190233E+06 | -0.04291368E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIH3NH2

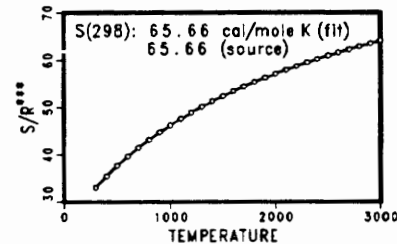
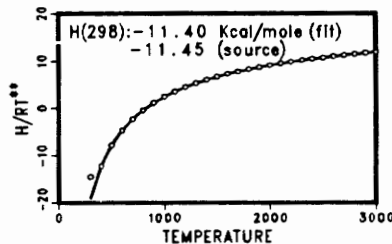
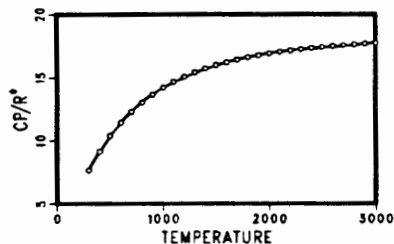
SILYLAMINE

GAS

As of: 4/24/89

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6              | a7              |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.02936348E+02 | 0.16747041E-01 | -0.03232858E-05 | -0.09171970E-07 | 0.03979516E-10 | -0.07334716E+05 | 0.11414373E+02  |
| 1000-3000K   | 0.08109945E+02 | 0.07215752E-01 | -0.06052251E-05 | -0.07086088E-08 | 0.15578638E-12 | -0.08999782E+05 | -0.16516504E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIH3NHSIH3

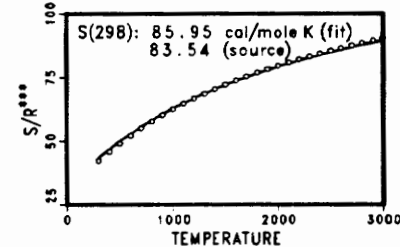
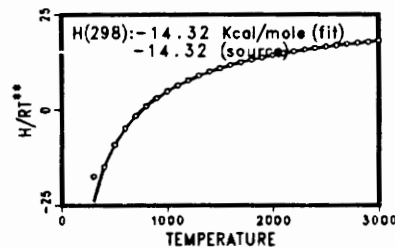
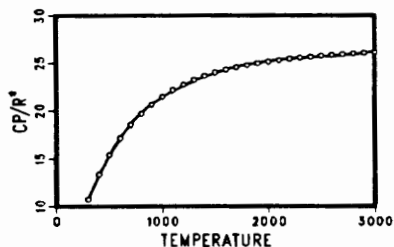
DISILYLAMINE

GAS

As of: 4/24/89

Fit

| Coefficients | a1             | a2             | a3              | a4              | a5             | a6              | a7              |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.02468749E+02 | 0.02940254E+00 | -0.06248179E-05 | -0.01731461E-06 | 0.07545261E-10 | -0.09209690E+05 | 0.02059559E+03  |
| 1000-3000K   | 0.12652963E+02 | 0.10667481E-01 | -0.10073358E-05 | -0.10812221E-08 | 0.02452363E-11 | -0.12497210E+05 | -0.03441428E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIH3NSIH3

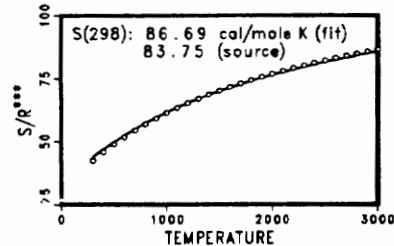
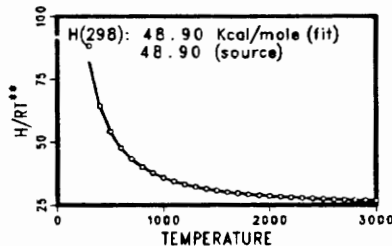
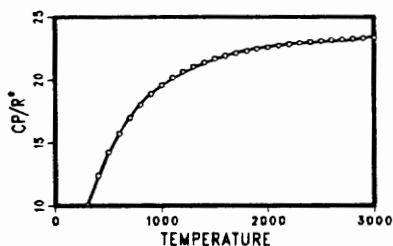
DISILYLAMIDOGEN

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.02827574E+02 | 0.02580646E+00 | -0.04200477E-05 | -0.15038588E-07 | 0.06388324E-10 | 0.02265351E+06 | 0.01997012E+03  |
| 1000-3000K   | 0.12014620E+02 | 0.09187517E-01 | -0.09159516E-05 | -0.09380967E-08 | 0.02156435E-11 | 0.01965065E+06 | -0.02978185E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIH4

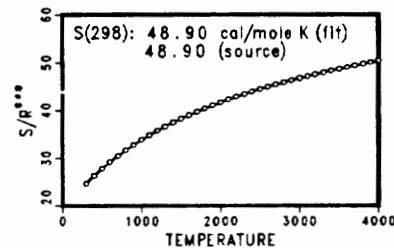
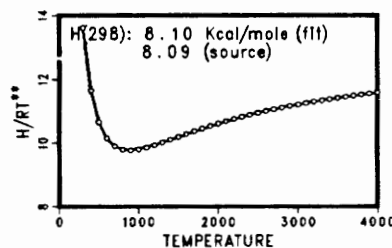
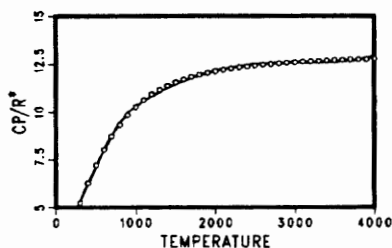
SILANE

GAS

As of: 12/13/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|----------------|-----------------|
| 0300-1000K   | 0.02475166E+02 | 0.09003721E-01 | 0.02185394E-04  | -0.02681423E-07 | -0.06621080E-11 | 0.02925488E+05 | 0.07751014E+02  |
| 1000-4000K   | 0.06893873E+02 | 0.04030500E-01 | -0.04183314E-05 | -0.02291394E-08 | 0.04384766E-12  | 0.11070374E+04 | -0.01749116E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIHCL2

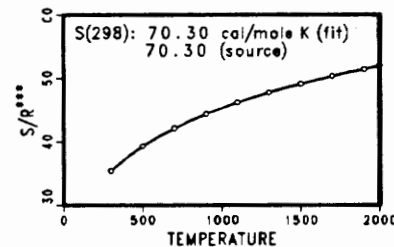
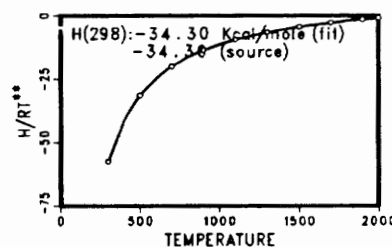
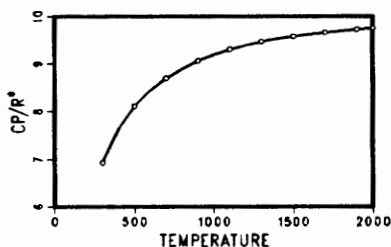
DICHLOROSILYL RADICAL

GAS

As of: 12/19/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02368353E+02 | 0.02401088E+00 | -0.03717219E-03 | 0.02851997E-06  | -0.08530494E-10 | -0.01875884E+06 | 0.16145866E+02  |
| 1000-2000K   | 0.07229734E+02 | 0.02869205E-01 | -0.08849876E-05 | -0.07495865E-09 | 0.05752338E-12  | -0.01971399E+06 | -0.07052663E+02 |



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIHF

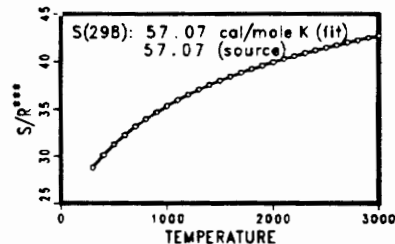
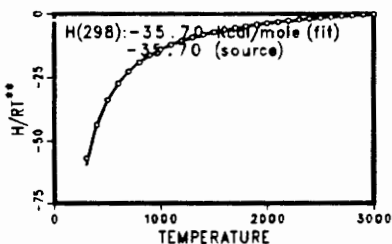
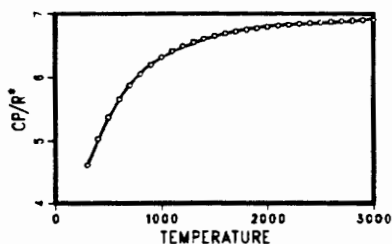
FLUOROSILYLENE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.03223727E+02 | 0.04981220E-01 | -0.03173051E-05 | -0.02822231E-07 | 0.12478316E-11 | -0.01914167E+06 | 0.08906423E+02  |
| 1000-3000K   | 0.05073508E+02 | 0.15332789E-02 | -0.01840658E-05 | -0.14400376E-09 | 0.03452517E-12 | -0.01973879E+06 | -0.10795069E+01 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: SIHF2

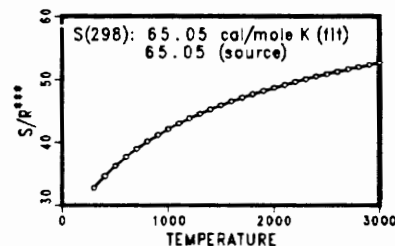
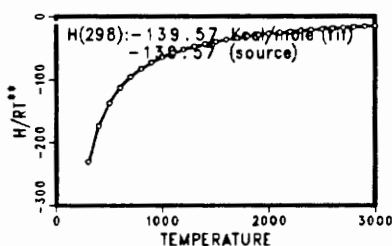
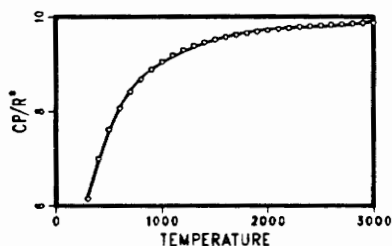
DIFLUOROSILYL

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.03377237E+02 | 0.10366072E-01 | -0.12390823E-05 | -0.07267981E-07 | 0.03794989E-10 | -0.07168358E+06 | 0.10521894E+02  |
| 1000-3000K   | 0.07216536E+02 | 0.02253240E-01 | -0.02737472E-05 | -0.02173460E-08 | 0.05255331E-12 | -0.07280241E+06 | -0.09783487E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

Species: SIHF3

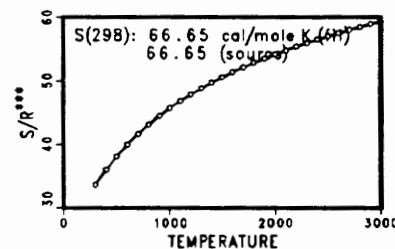
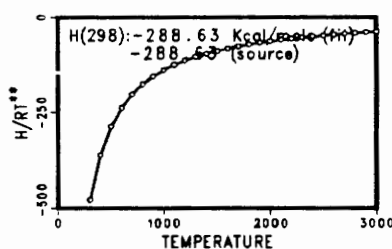
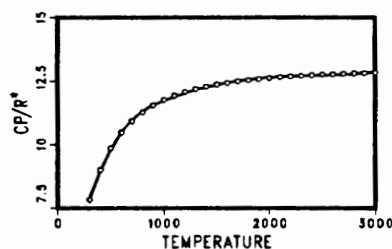
TRIFLUOROSILANE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|-----------------|-----------------|
| 0300-1000K   | 0.03918053E+02 | 0.14639172E-01 | -0.01856069E-04 | -0.10582003E-07 | 0.05617543E-10 | -0.14704386E+06 | 0.07024261E+02  |
| 1000-3000K   | 0.09363567E+02 | 0.02947555E-01 | -0.03577633E-05 | -0.02858224E-08 | 0.06915728E-12 | -0.14860736E+06 | -0.02169452E+03 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$



Species: SIN

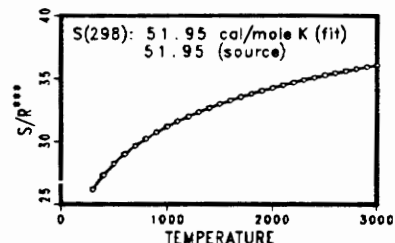
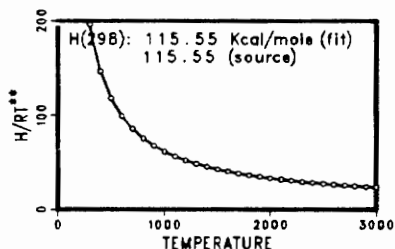
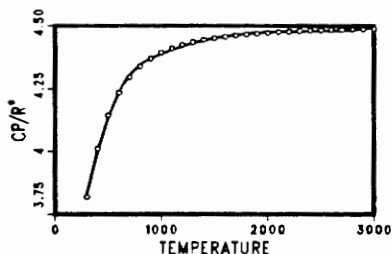
SILICON NITRIDE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|----------------|
| 0300-1000K   | 0.03149181E+02 | 0.02584376E-01 | -0.05804624E-05 | -0.01805626E-07 | 0.10410949E-11 | 0.05710563E+06 | 0.07474389E+02 |
| 1000-3000K   | 0.04122909E+02 | 0.03521457E-02 | -0.07161080E-06 | -0.02154956E-09 | 0.06667570E-13 | 0.05683927E+06 | 0.02389837E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

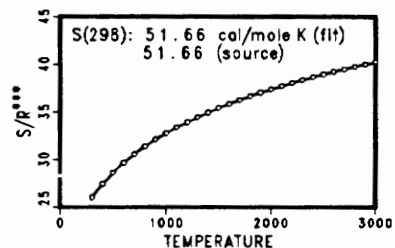
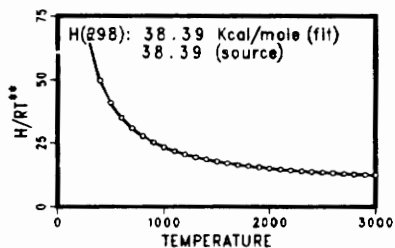
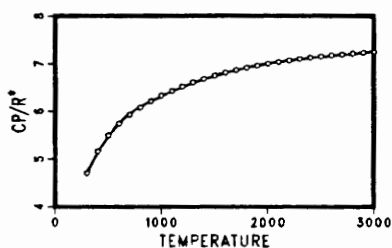
Species: SINH

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03166974E+02 | 0.05805822E-01 | -0.09524443E-05 | -0.03991892E-07 | 0.02283188E-10 | 0.01813560E+06 | 0.06298439E+02  |
| 1000-3000K   | 0.04928800E+02 | 0.16286244E-02 | -0.13671971E-06 | -0.13904604E-09 | 0.02998968E-12 | 0.01767789E+06 | -0.02823472E+02 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SINH2

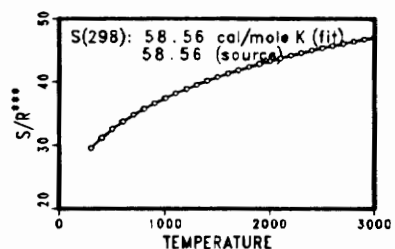
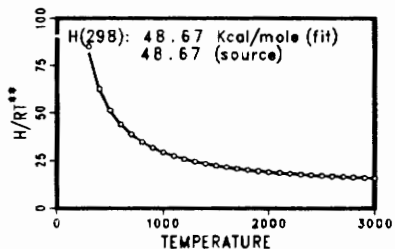
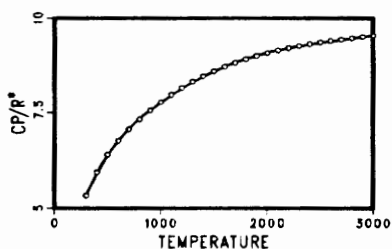
AMINOSILYLIDYNE

GAS

As of: 4/24/89

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub> | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|
| 0300-1000K   | 0.03362769E+02 | 0.07261175E-01 | -0.08721233E-05 | -0.04400014E-07 | 0.02419532E-10 | 0.02318445E+06 | 0.08223867E+02  |
| 1000-3000K   | 0.05186435E+02 | 0.03016656E-01 | -0.02165476E-05 | -0.02722658E-08 | 0.05706182E-12 | 0.02270507E+06 | -0.12421399E+01 |



Source: SNLL FIT TO BAC-MP4 DATA

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SN

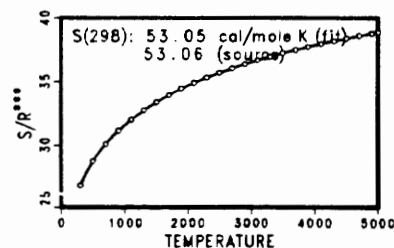
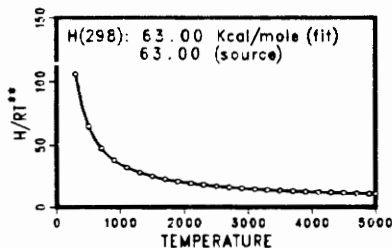
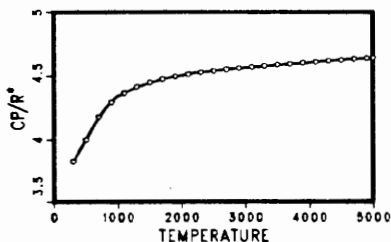
SULFUR NITRIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub> | a <sub>7</sub> |
|--------------|----------------|----------------|-----------------|----------------|-----------------|----------------|----------------|
| 0300-1000K   | 0.03407345E+02 | 0.01797887E-01 | -0.02018969E-04 | 0.02107857E-07 | -0.09527593E-11 | 0.03062373E+06 | 0.06821481E+02 |
| 1000-5000K   | 0.03888286E+02 | 0.06778427E-02 | -0.02725308E-05 | 0.05135927E-09 | -0.03593836E-13 | 0.03044496E+06 | 0.04194291E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SO

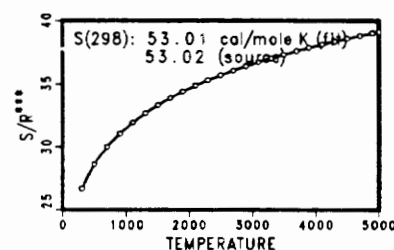
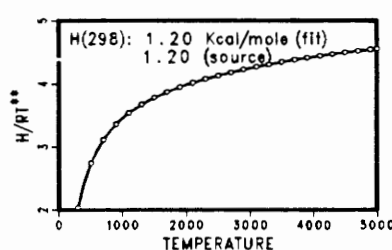
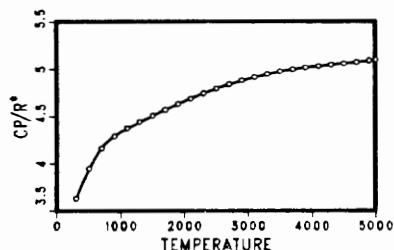
SULFUR MONOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub> | a <sub>4</sub>  | a <sub>5</sub> | a <sub>6</sub>  | a <sub>7</sub> |
|--------------|----------------|----------------|----------------|-----------------|----------------|-----------------|----------------|
| 0300-1000K   | 0.03080401E+02 | 0.01803105E-01 | 0.06705022E-05 | -0.02069005E-07 | 0.08514657E-11 | -0.03986163E+04 | 0.08581028E+02 |
| 1000-5000K   | 0.04021077E+02 | 0.02584856E-02 | 0.08948142E-06 | -0.03580144E-09 | 0.03228430E-13 | -0.07119620E+04 | 0.03452522E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SO2

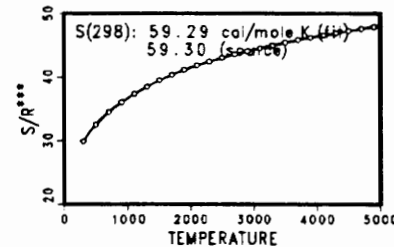
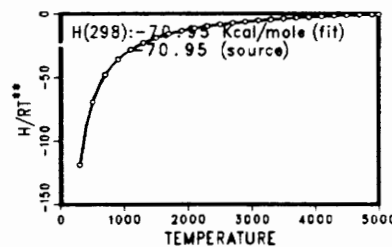
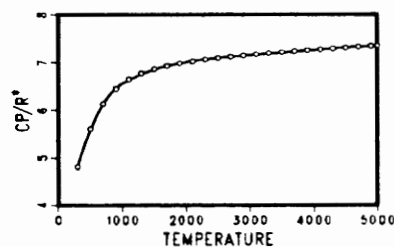
SULFUR DIOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a <sub>1</sub> | a <sub>2</sub> | a <sub>3</sub>  | a <sub>4</sub> | a <sub>5</sub>  | a <sub>6</sub>  | a <sub>7</sub>  |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02911438E+02 | 0.08103022E-01 | -0.06906710E-04 | 0.03329015E-07 | -0.08777121E-11 | -0.03687881E+06 | 0.11117403E+02  |
| 1000-5000K   | 0.05254498E+02 | 0.01978545E-01 | -0.08204226E-05 | 0.15763830E-09 | -0.11204512E-13 | -0.03756885E+06 | -0.11460563E+01 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SO3

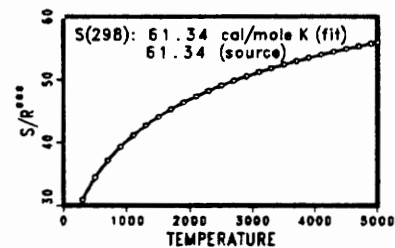
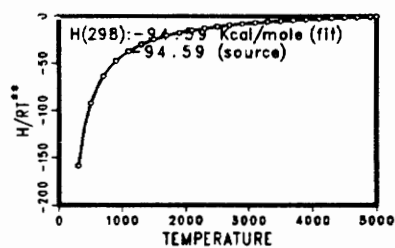
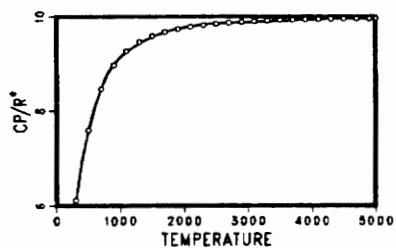
SULFUR TRIOXIDE

GAS

As of: 12/12/86

Fit

| Coefficients | a1             | a2             | a3              | a4             | a5              | a6              | a7              |
|--------------|----------------|----------------|-----------------|----------------|-----------------|-----------------|-----------------|
| 0300-1000K   | 0.02575282E+02 | 0.15150916E-01 | -0.12298717E-04 | 0.04240257E-07 | -0.05266812E-11 | -0.04894410E+06 | 0.12195116E+02  |
| 1000-5000K   | 0.07050668E+02 | 0.03246560E-01 | -0.14088974E-05 | 0.02721535E-08 | -0.01942364E-12 | -0.05020667E+06 | -0.11064426E+02 |



Source: SNLL FIT TO JANAF TABLES

$$* CP/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$** H/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7$$

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